GAMMA

Graphics Documentation

$$\hat{\hat{\Gamma}}$$

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Date:	May 22, 1998

Graphics Chapters

1 Introduction

This document discusses the ways in which GAMMA can be used to both input and output data in formats suitable for processing and/or the production of graphical plots. Actual plotting is inevitably done using **OTHER** software. Thus, GAMMA only serves as a hub which manipulates data. There are three data types in GAMMA which are often used to contain information that is to be displayed graphically. These are row vectors, matrices, and coordinate vectors.

GAMMA Supported I/O

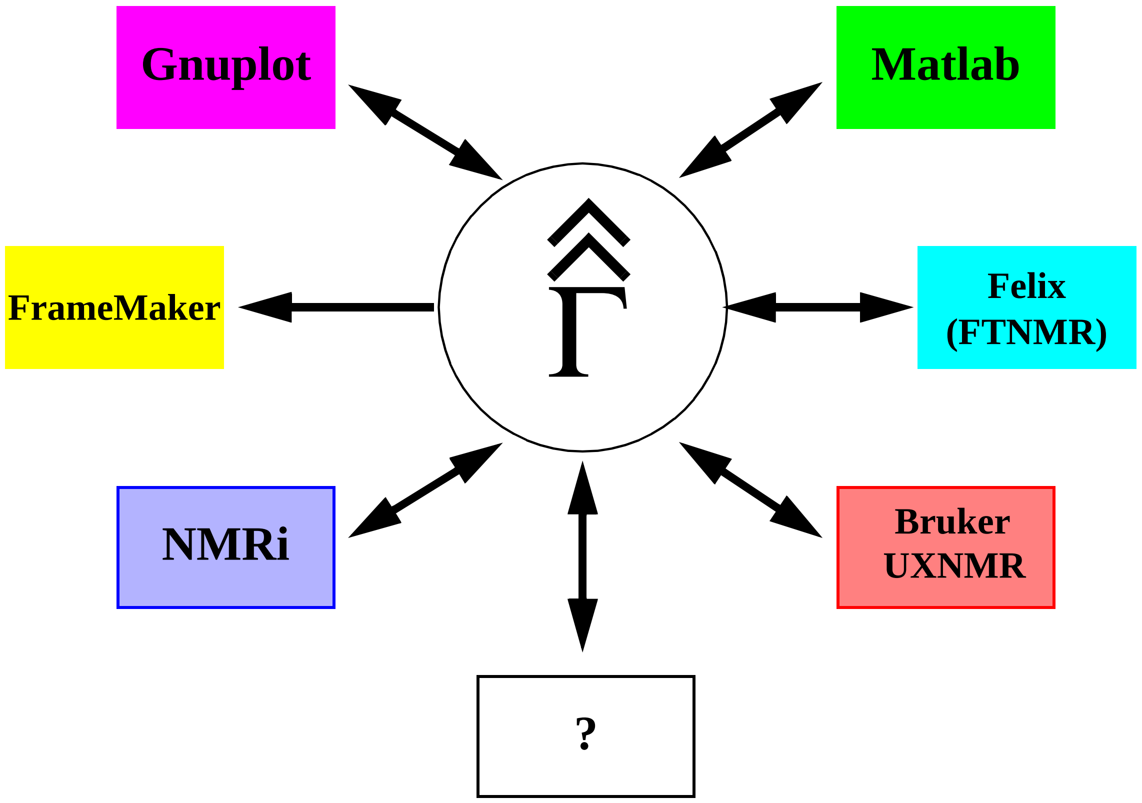


Figure 19-1 : Some of the programs with which GAMMA can easily interact. There are other prgrams that also have been used with GAMMA, those that come to mind at the moment are SigmaPlot, Deltagraph and XMGR. These take ASCII input and need no special interface.

2 Gnuplot Output

2.1 Overview

Gnuplot is a plotting package which runs on Unix systems, PCs and Macs. It's price (free) and versatility make it a good choice for use in visualization of data. GAMMA's Gnuplot routines are provided to allow the output of vector, matrix, and coordinate vector data into ASCII files suitable for plotting in Gnuplot. Aside from being able to see your simulation result plotted on virtually every kind of computer you are using, Gnuplot also allows one to build **interactive** GAMMA programs that plot to the screen. Furthermore, Gnuplot can output plots in many different formats and to many different types of devices. More information regarding the software can be found at **http://www.cs.dartmouth.edu/gnuplot_info.html**.

2.2 Available Gnuplot Functions

2.3 Index of Figures & Tables

2.4 Routines

2.4.1 GP_1D

Usage:

```
#include <gnuplot.h>
void GP_1D (const char* filename, const row_vector& vx, int ri=0,
                                double xmin=0, double xmax=0, double cutoff=0);
void GP_1D (ofstream& ofstr, const row_vector& vx, int ri=0,
                                double xmin=0, double xmax=0, double cutoff=0);
```

Description:

The function ***GP_1D*** writes the information contained in the input row vector **vx** in ASCII format to either a file or a file stream. The integer flag **ri** dictates whether real (ri=0, default), imaginary (ri<0), or complex values from vx will be output. If **xmax** or **xmax** & **xmin** are specified the horizonatal axes will be labeled, the first point with the value of **xmin** and the last point with the value of **xmax**. For some 1D plots, points in the Gnuplot output file may be skipped and hence (from smooth data) the output file size reduced. This is done automatically by this GAMMA function, the value of **cutoff** indicative of what point variation is considered roundoff. Note that some type of plotting do not allow for skipped points and the value of **cutoff** should be left at zero. The latter form of the function is useful for successive writes of 1D spectra to the same file.

Return Value:

Nothing. A new disk file in ASCII is produced for plotting with Gnuplot (or other plotting programs which take ASCII). It will contain either one or two plots depending on the flag “rc”.

Example:

```
#include <gamma.h>
main ()
 {
 int npts=101;                          // How about this many points
 row_vector data(npts);                 // 1-dim. data block
 double x, y;                           // Some temporary variables
 for(int i=0; i<npts; i++)               // Fill up data block
  {
  x = double(i-50);
  y = x*x*x/125000;                     // Cubical parabolic in imaginaries
  x = x*x/2500;                         // Regular parabolic into reals
  data.put(complex(x,y),i);             // Put this point into the vector
  }
 GP_1D("real.gnu", data, 0);            // Write real points to an ASCII file
 GP_1D("imag.gnu", data, -1);           // Write imaginary points to an ASCII file
 GP_1D("bides.gnu", data, 1);           // Write complex points to anASCII file
```

```
        }
```

When compiled and executed, the program makes three ASCII files suitable for use in Gnuplot They may be readily viewed with that program or used in any other plotting program that takes ASCII input. The following dialog demostrates how to display these plots on the screen on a Unix system (assuming Gnuplot is installed and the executable "gnuplot" is in the users path).

```
|gamma1>gnuplot
  G N U P L O T
  unix version 3.5
  patchlevel 3.50.1.17, 27 Aug 93
  last modified Fri Aug 27 05:21:33 GMT 1993
  Copyright(C) 1986 - 1993   Colin Kelley, Thomas Williams
  Send comments and requests for help to info-gnuplot@dartmouth.edu
  Send bugs, suggestions and mods to bug-gnuplot@dartmouth.edu
  Terminal type set to 'x11'
  gnuplot> set data style lines
  gnuplot> plot "real.gnu"
  gnuplot> plot "imag.gnu"
  gnuplot> plot "bides.gnu"
  gnuplot> quit
|gamma1>
```

Since this documentation was created with the program FrameMaker, I can also put these plots directly into the document. For example, before the "quit" command above I can do the following

```
gnuplot> set terminal mif
Terminal type set to 'mif'
Options are 'colour polyline'
gnuplot> set output "real.mif"
gnuplot> plot "real.gnu"
```

This produces three corresponding MIF files that are shown in the next figure. Other than being resized, they have not been altered within FrameMaker (although they could be.)

Gnuplot Funcion GP_1D Example

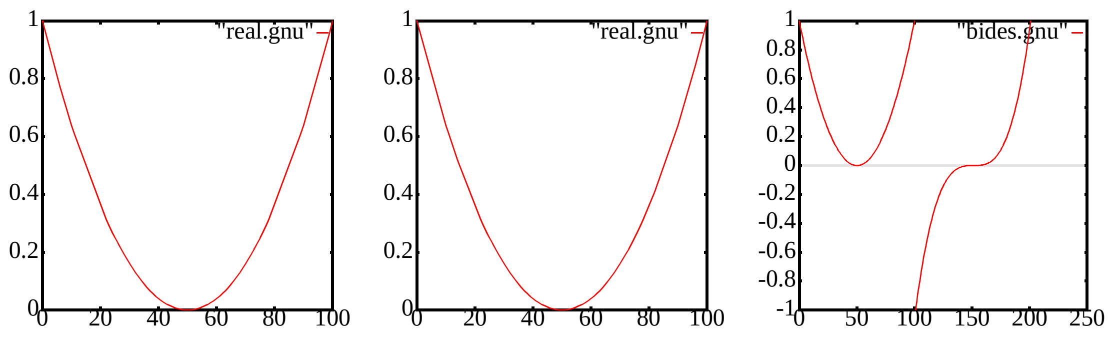


Figure 4-1 - Example program result from use of the GAMMA function “Felix”.

See Also:

2.4.2 GP_1Dm

Usage:

```
#include <gnuplot.h>
void GP_1Dm(const String& filename, row_vector* vx, int N,
                                        int ri=0, double xmin=0, double xmax=0, int cutoff =0);
```

Description:

The function ***GP_1Dm*** creates an ASCII file called **filename** suitable for reading and plotting with Gnuplot. It will contain plot(s) of the data contained in the array of vectors **vx** on the y-axis versus point number on the x-axis. The number of vectors (in the array **vx**) to plot is given by the integer **N**. The x-axis produced will span a range [**xmin**, **xmax**] which defaults to [0,1]. The flag "**ri**" dictates which plot(s) are produced. For rc = 0 (default) only the real data is plotted. For rc < 0 only the imaginary data is plotted. For rc>0, both the real and imaginary plots are produced. For some 1D plots, points in the Gnuplot output file may be skipped and hence (from smooth data) the output file size reduced. This is done automatically by this GAMMA function, the value of **cutoff** indicative of what point variation is considered roundoff. Note that some type of plotting do not allow for skipped points and the value of **cutoff** should be left at zero.

Return Value:

Nothing. A new disk file in ASCII is produced for plotting with Gnuplot (or other plotting programs which take ASCII). It will contain one or more plots depending on the value of N.

Example:

```
#include <gamma.h>
main ()
 {
 int i, npts=101;                              // Temp index, # points
 row_vector data[3],  datatmp(npts);           // Vector array, temp. vector
 for(i=0; i<3; i++) data[i] = datatmp;         // Initialize vectors in array
 double x;                                     //Temp variable
 for(i=0; i<npts; i++)                         // Fill up data blocks
  {
  x = double(i-npts/2);                        //      The "x" value
  data[0].put(x*x/2500.0,i);                   //      The "y" value, 1st vector
  data[1].put(x*x*x/12500.0,i);                //      The "y" value, 2nd vector
  data[2].put(x*x*x*x/312500.0,i);             //      The "y" value, 3rd vector
  }
 GP_1Dm("plots.asc", data, 3);                 // Write real points to ASCII file
 cout << "\n\n";                               // Keep the screen nice
 }
```

Gnuplot Function GP_1Dm Example

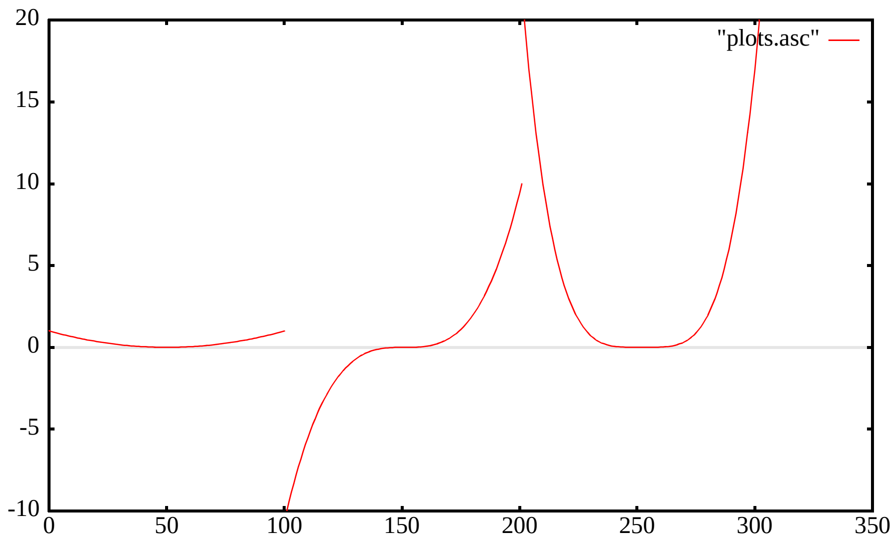


Figure 4-2 - Example program result from use of the GAMMA function “GP_1Dm”.

The plot above was incorporated directly into this file using the “MIF” export type in Gnuplot. After the plot is displayed on the screen, the commands *set terminal MIF, set output “plot.mif”*, and *replot* were given to have Gnuplot produce the plot in MIF format in the file plot.mif. The file plot.mif was imported to this document with the FrameMaker import command under the File option.

See Also:

2.4.3 GP_xy

Usage:

```
#include <gnuplot.h>
void GP_xy (const char* filename, const row_vector &vx);
void GP_xy (ofstream& ofstr, const row_vector &vx);
```

Description:

The function GP_xy creates an ASCI file “filename” in a format suitible for use in Gnuplot. Unlike function GP_1D which assumes the data is monotonically increasing on the horizontal axis, GP_xy produces plots in parametric fashion, i.e. true x *versus* y. The plot will be of the data supplied by the vector vx. It is recommended that “filename” end with “.asc” to signify an ASCII file.

Return Value:

Nothing. A new disk file is produced for use in Gnuplot.

Example:

```
#include <gamma.h>
main ()
   {
   row_vector data(360);                        // Create a data block
   double x,y,theta;                            // Declare needed variables
   for(int i=0; i<360; i++)                     // Loop through 360 degrees
      {                                         // Fill up block with Astroid
      theta = i*2.0*PI/360.0;                   // also called a Hypercycloid of four cusps
      x = cos(theta);                           // x = a*[cos(theta)]**3, here a = 1
      y = sin(theta);                           // y = a*[sin(theta)]**3, here a = 1
      x = x*x*x;
      y = y*y*y;
      data.put(complex(x,y), i);                // Store the data point
      }
   GP_xy("astroid.asc", data);                  // Output Gnuplot .mif plot file
  GP_xyplot("asteroid.gnu", "astroid.asc");     // Interacitvely plot to screen!
 }
```

Gnuplot Function GP_xy Example

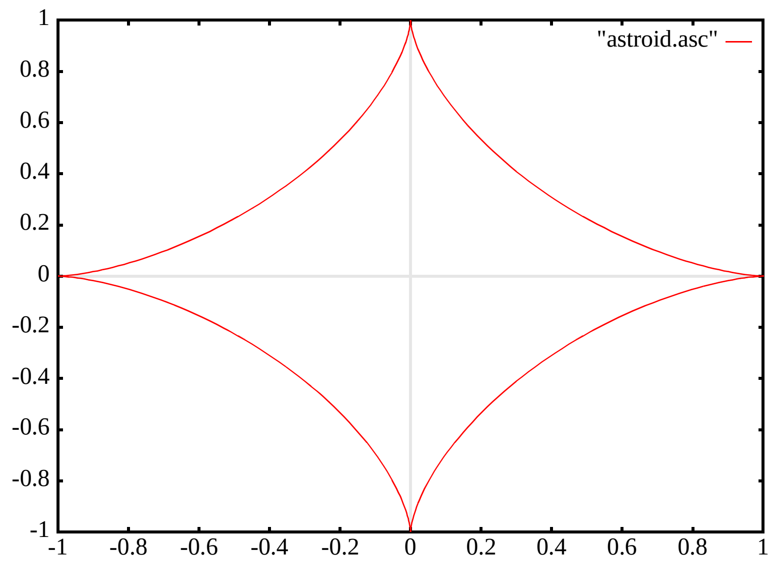


Figure 4-3 - Example program result from use of the GAMMA function “GP_xy”.

The plot above was incorporated directly into this file using the “MIF” export type in Gnuplot. After the plot is displayed on the screen, the commands *set terminal MIF, set output “plot.mif”*, and *replot* were given to have Gnuplot produce the plot in MIF format in the file plot.mif. The file plot.mif was imported to this document with the FrameMaker import command under the File option.

See Also: GP_1D, GP_1Dm

2.4.4 GP_contour

Usage:

```
#include <gnuplot.h>
void GP_contour(ofstream& ofstr, const row_vector& vx, double row,
                                   int row_inc=0, double xmin=0, double xmax=0, double cutoff=0)
void GP_contour(ofstream& ofstr, matrix& mx,
             int row_inc=0, double ymin=0, double ymax=0, double double xmin=0, double xmax=0)
void GP_contour(ofstream& ofstr, matrix& mx, double row,
             int row_inc=0, double ymin=0, double ymax=0, double double xmin=0, double xmax=0)
```

Description:

The functions ***GP_contour*** is used to create contour plots in Gnuplot MIF format.

FM_contour (const char* filename, matrix &mx, double threshold, int steps, double CLI, double CLM, int CPN, double xsize, double ysize) -The function FM_contour creates a Gnuplot file called filename in the MIF format. The produced file will contain a contour plot of the real data contained in the matrix mx. The contours begin at the level set by threshold and increment by the value of CLI. The number of contours is set by steps. The levels increment either geometrically or linearly as set by the value of CLM, the default is linear. Positive and negative contours are set by the flag CPN. For CPN=1 (default), both positive and negative contours are produced. For CPN=0 only the positive contours are output while for CPN=-1 only the negative contours are done. The output file contour plot will be of dimension xsize by ysize (both given in centimeters, default 10 cm).

CPN - This is a flag to indicate whether positive (or increasing), negative (or decreasing), or both positive and negative contours. If CPN = 0, only contours increasing from the set threshold will be computed. If CPN = -1 only contours decreasing from the set threshold will be computed. If CPN = 1 (default), contour will be computed increasing from |threshold| and decreasing from -|threshold|.

xsize, ysize - These determine the overall plot dimensions the Gnuplot output will assume. The values are input in centimeters and are defaulted to 10 cm each. The values do nothing to the relative x to y scaling implicit in the data matrix, thus a 256 by 512 array will be 5 x 10 cm even though xsize and ysize are both set to 10 cm.

Return Value:

Nothing. A new disk file is produced for incorporation into Gnuplot.

Example:

```
#include <gamma.h>
main()
  {
  matrix mx(101,101);                        // Data matrix
  row_vector vx1(101), vx2(101);             // Two working blocks of length 101
  vx1 = sinc(101, 50, 10);                   // Use provided window sinc function
  vx2 = sin_square(101, 50);                 // Use provided window sin squared function
  for(int i=0; i<101; i++)                   // Loop through and fill up the matrix
    for(int j=0; j<101; j++)
      mx.put(vx1.get(i)*vx2.get(j),i,j);
  String afile = "contour.asc";              // Output ASCII file name
  GP_contour(afile, mx);                     // Write the ASCII file for Gnuplot
  GP_contplot("contour.gnu", afile);         // Interactively output contour plot
  }
```

Gnuplot Function GP_contour Example

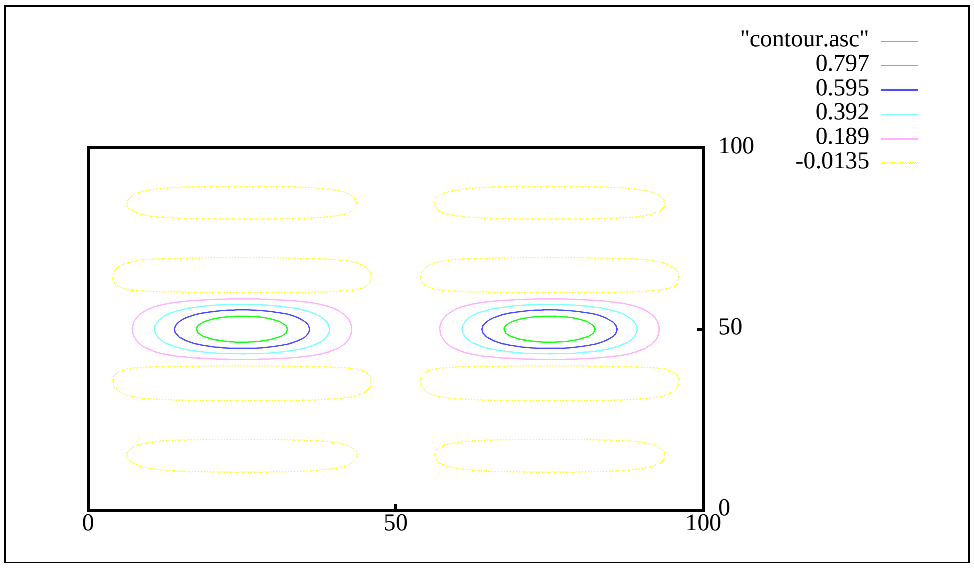


Figure 4-4 - Example program result from use of the GAMMA function “GP_stack”.

See Also: FM_stack

2.4.5 GP_stack

Usage:

```
#include <gnuplot.h>
void GP_stack(ofstream& ofstr, const& row_vector, double row,
                                        int row_inc, double xmin, double xmax, double cutoff=0)
void GP_stack(String& filename, matrix& mx,
             int row_inc=0, double ymin=0, double ymax=0, double double xmin=0, double xmax=0)
void GP_stack(ofstream& ofstr, matrix& mx, double row,
                                        int row_inc, double xmin, double xmax, double cutoff=0)
```

Description:

The function GP_stack creates an ASCII file Gnuplot file called “filename” in the MIF format. It contains a single stack plot of dimension xsize by ysize (both given in centimeters, default 14 cm). The data is input in the form of a matrix and the plot is of the entire matrix real data. The values xinc and yinc, also given in centimeters, are the amount to shift the next row in the horizontal and vertical directions respectively. The rows which are to be plotted are specified by the value row_inc, e.g. a row increment of 3 causes the first, fourth, seventh, etc., until the end of the matrix is reached.

Return Value:

Nothing. A new disk file is produced for incorporation into Gnuplot.

Example:

```
#include <gamma.h>
main()
  {
  matrix mx(101, 101);                // Create a 101x101 matrix for data
  row_vector vx(100);                 // Create a 1D-data block of length 101
  vx = sinc(101, 50, 10);             // Use provided window sinc function
  for(int i=0; i<101; i++)            // Loop through and fill up the matrix
   for(int j=0; j<101; j++)
     mx(i,j) = vx(i) * vx(j);
  String afile = "stack.asc";         // Output ASCII file name
  GP_stack(afile, mx);                // Write the ASCII file for Gnuplot
  }
```

This example generates a 101x101 matrix which is a sinc function along both axes.

The following dialog demostrates how to display these plots on the screen on a Unix system (assuming Gnuplot is installed and the executable “gnuplot” is in the users path).

```
|gamma1>gnuplot
  G N U P L O T
```

```
unix version 3.5
patchlevel 3.50.1.17, 27 Aug 93
last modified Fri Aug 27 05:21:33 GMT 1993
Copyright(C) 1986 - 1993   Colin Kelley, Thomas Williams
Send comments and requests for help to info-gnuplot@dartmouth.edu
Send bugs, suggestions and mods to bug-gnuplot@dartmouth.edu
Terminal type set to ’x11’
gnuplot> set data style lines
gnuplot> set parametric
gnuplot> splot "stack.asc"
```

Since this documentation was created with the program FrameMaker, I can also put these plots directly into the document. For example, before the “quit” command I can do the following

```
gnuplot> set terminal mif
Terminal type set to 'mif'
Options are 'colour polyline'
gnuplot> set output "stack.mif"
gnuplot> replot
gnuplot> quit
```

This produces a MIF files that is shown in the next figure. Other than being resized, is has not been altered within FrameMaker (although it could be.)

Gnuplot Function GP_stack Example

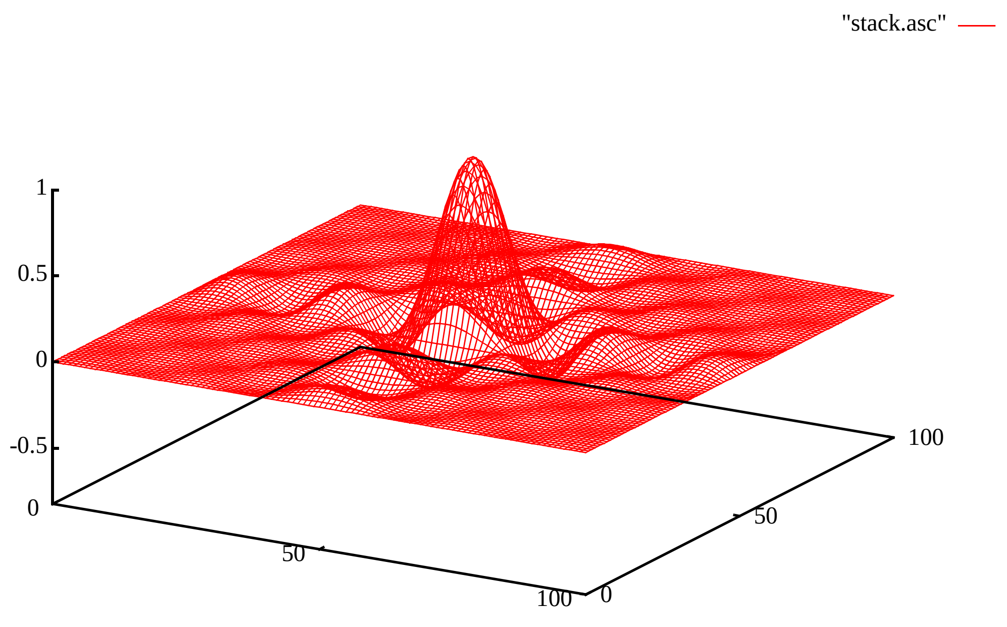


Figure 4-5 - Example program result from use of the GAMMA function “GP_stack”.

2.5 Routines for Interactive Plotting Using Gnuplot

2.5.1 GP_1Dplot

Usage:

```
#include <gnuplot.h>
void GP_1Dplot(const String& gnumacro, const String& file1D, int join = 1);
void GP_1Dplot(GPdat& G);
```

Description:

The function ***GP_1Dplot*** can be used to produce 1D plots to the screen while a GAMMA program is running using Gnuplot. This is in three steps. First, during the course of a simulation, an ASCII file suitable for use in Gnuplot is written to a file. Second, an ASCII file full of Gnuplot commands to plot the ASCII data file is written to another file. Finally, Gnuplot is invoked and the commands executed.

Return Value:

Nothing. A new disk file in the MMF is produced for incorporation into Gnuplot.

Example:

```
#include “gamma.h”

FM_Matrix (“Testa1.mmf”,c);
}
( 6.00, 6.00)
```

Note that the 1,1 is set to the integer 1, the 1,2 element to 1.00 because its full value is 1.001. The imaginary part has a value of 0.0001 and falls below threshold.

See Also: FM_Mat_Plot

2.6 Additional Examples

2.6.1 Spherical Plots

Description:

Although there is no function in GAMMA (yet) to support it directly, users can make 3D spherical plots with Gnuplot and GAMMA. In this instance the program should generate a coordinate vector of the 3D points. These are subsequently projected into 2 dimensions with the coordinate vector projection function. The GP_xy function is then used to output the projected points.

Example:

```
#include <gamma.h>
main (int argc, char** argv)
 {
 iint N = 4096;                         // We’ll plot this many points
   coord_vec data(N);                   // Here’s a coordinate vector
   double x, y, z;                       // Here are ordinates
   double w, W = 250.0;
   double Nm1 = double(N-1);
   double di;
   for(int i=0; i<N; i++)               // Now we’ll fill up the vector
     {
     di = double(i);                    //     Point value
     w = W*di/Nm1;                      //     Frequency vlaue
     z = -1.0 + 2.0*di/Nm1;             //     Let z = [-1, 1]
     x = sin(w);                        //     Take x oscillating
     y = cos(w);                        //     Take y oscillating
     data.put(x,y,z,i);                 //     Store coordinate
     }
   row_vector proj(N);                  // For projected data
   double TH, PH;
   double fact = 180.0/PI;
   coord pt;
   for(int l=0; l<N; l++)
     {
     pt = data(l);
     TH =  fact*pt.theta();
     PH = fact*pt.phi();
     proj.put(complex(PH,90-TH),l);
```

```
      }
    GP_xy("sphere.asc", proj);                    // 2D gnuplot of traj
    cout << "\n\n";                               // Keep the screen nice
  }
```

This plot makes a helix which spirals up the surface of a sphere. The following dialog demostrates how to display these plots on the screen on a Unix system (assuming Gnuplot is installed and the executable “gnuplot” is in the users path).

```
|gamma1>gnuplot
  G N U P L O T
  unix version 3.5
  patchlevel 3.50.1.17, 27 Aug 93
  last modified Fri Aug 27 05:21:33 GMT 1993
  Copyright(C) 1986 - 1993   Colin Kelley, Thomas Williams
  Send comments and requests for help to info-gnuplot@dartmouth.edu
  Send bugs, suggestions and mods to bug-gnuplot@dartmouth.edu
  Terminal type set to 'x11'
  gnuplot> set data style line
  gnuplot> set parametric
    dummy variable is t for curves, u/v for surfaces
  gnuplot> set angles degrees
  gnuplot> set title "3D Trajectory"
  gnuplot> set nokey
  gnuplot> set view 80,140,.6, 2.5
  gnuplot> set mapping spherical
  gnuplot> set samples 32
  gnuplot> set isosamples 9
  gnuplot> set urange [-pi/2:pi/2]
  gnuplot> set vrange [0:2*pi]
  gnuplot> splot cos(u)*cos(v),cos(u)*sin(v),sin(u) with lines 3 4, 'sphere.asc' with lines 1 2
  gnuplot> set terminal mif
    Terminal type set to 'mif'
    Options are 'colour polyline'
  gnuplot> set output "x.mif"
  gnuplot> replot
  gnuplot> quit
```

The last lines produce a MIF file that is shown in the next figure. Other than being resized, is has not been altered within FrameMaker (although it could be.)

Gnuplot 3D Spherical Plot Example

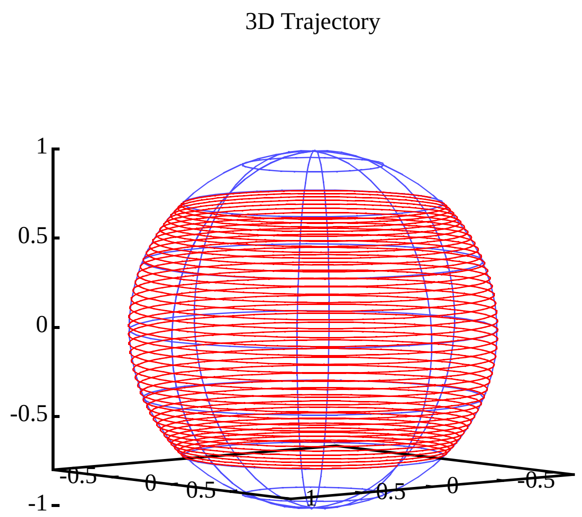


Figure 4-6 - Example program result illustrating production of 3D spherical plots.

2.7 Additional Hints

2.7.1 Gnuplot Contour Plots

The contouring function takes a GAMMA matrix and slices through specified contours to produce a Gnuplot MIF output file. An attempt is made to group all points for each specific contour line

2.7.2 Gnuplot Stack Plots

The contouring function takes a GAMMA matrix and slices through specified contours to produce a Gnuplot MIF output file. An attempt is made to group all points for each specific contour line

3 FrameMaker Output

Sections In This Document

3.1 FrameMaker Overview

The FrameMaker output routines are provided to allow the transfer of simulated plot data into FrameMaker compatible files. This is highly useful for the preparation of documents which are to contain plots of your GAMMA simulated spectra. FrameMaker has the ability to blend text, equations, and graphics. Using GAMMA's FrameMaker routines, one may quickly produce publication quality documents, transparencies, HTML pages, etc.. that contain simulated spectra directly.

Since FrameMaker also has the ability to graphically manipulate GAMMA generated files, your plots may be cosmetically enhanced. Because GAMMA is capable of reading other file formats, it can serve a a conversion tool. If plot files from other programs are read into GAMMA (e.g. a matrix from Felix), they may be re-output into FrameMaker format for use in a document. FrameMaker can also be used just for viewing GAMMA simulated spectra on the screen.

GAMMA & FrameMaker

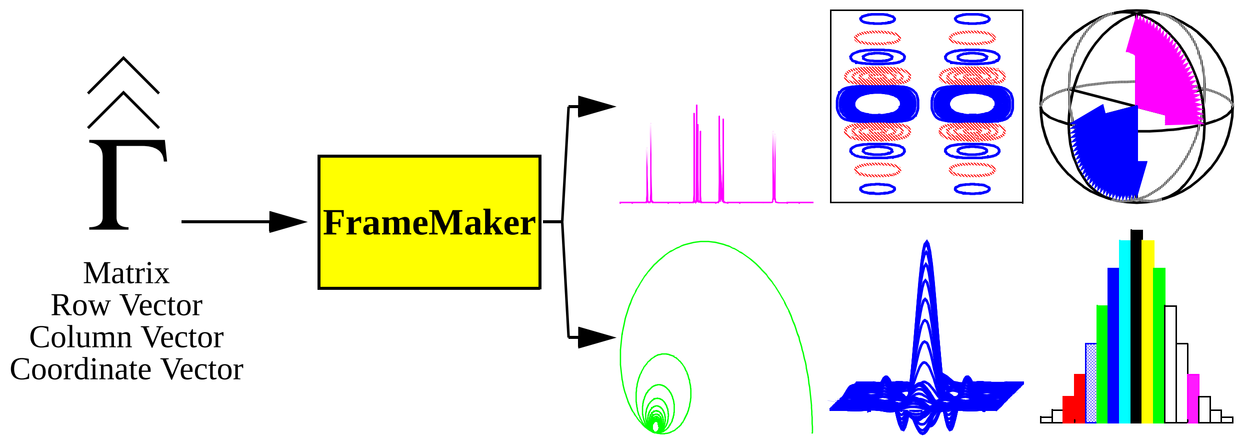


Figure 4-1 : GAMMA output in FrameMaker. You're viewing a document produced with FrameMaker and the plots were made with GAMMA.

Note that this is a ***one directional process***! Unlike other output formats supported by GAMMA (Felix, NMRi, etc.), GAMMA cannot re-read FrameMaker files. DO NOT make the mistake of considering your FrameMaker output files as a means of data storage from which further mathematical manipulations may be performed within GAMMA. FrameMaker files are exclusively used for FrameMaker.

A primary reason for GAMMA's interface to FrameMaker is that such plots are graphic objects. That is to say, they may be manipulated graphically inside FrameMaker. Your plots can be resized, recolored, annotated, added into other documents, made into transparencies, etc. The downside of this is that to use these routines you must purchase FrameMaker. More information regarding the software can be found at http://www.frame.com.

3.2 Index of GAMMA’s FrameMaker Functions

3.3 Index of Figures & Tables

3.4 FrameMaker Functions

3.4.1 FM_1D

Usage:

```
#include <FrameMaker.h>
void FM_1D (const char* filename, row_vector vx, double xsize=14,
                                        double ysize=14, double min=0, double max=1, int rc=0);
```

Description:

The function ***FM_1D*** creates a FrameMaker file called ***filename*** in the MIF format. It will contain plot(s) of the data contained in the vector ***vx*** on the y-axis versus point number on the x-axis. The plot(s) will be of dimension xsize by ysize in centimeters (default to 14x14 cm plot). The x-axis produced will span a range [***min***, ***max***] which defaults to [0,1]. The flag ***rc*** dictates which plot(s) are produced. For ***rc = 0*** (default) only the real data is plotted. For ***rc < 0*** only the imaginary data is plotted. For ***rc>0***, both the real and imaginary plots are produced. FrameMaker MIF files are typically named with a ".mif" suffix so it is recommended that all filenames used for this function end with .mif.

Return Value:

Nothing, a new disk file in the MIF is produced for incorporation into FrameMaker. It will contain either one or two plots depending on the flag "rc".

Example:

```
#include <gamma.h>
main ()
 {
 row_vector vx(101);                        // Block for data points
 double x, y;                               // Working x,y ordinates
 for(int i=0; i<101; i++)                   // Fill up data block
  {
  x = double(i-50);                         // Offset x (so centered)
  y = x*x*x/125000;                         // Cubical parabolic (imag)
  x = x*x/2500;                             // Parabolic into reals
  vx.put(complex(x,y),i);                   // Store this point
  }
 FM_1D("FM.mif",BLK,10,5, -50, 50, 1);      // Output FM.mif, both plots
 }
```

FM_1D Example Output

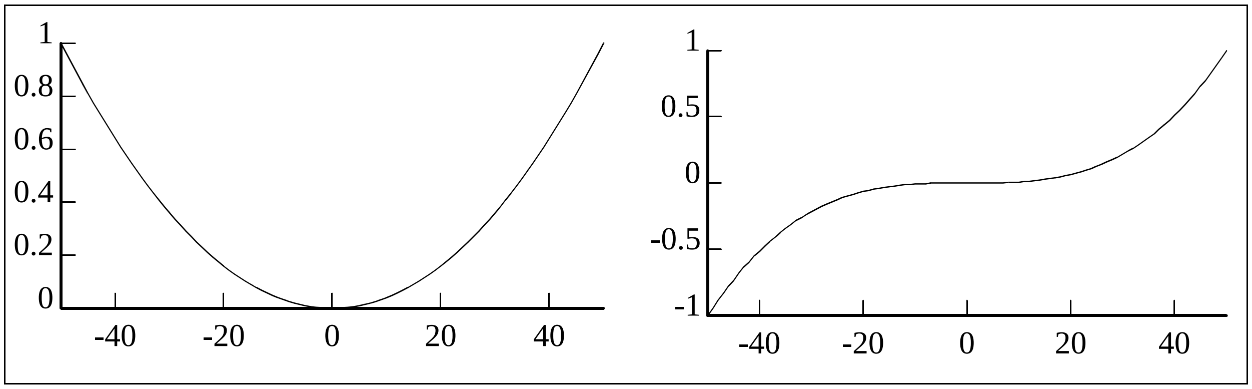


Figure 4-2 - The two plots above were contained in the file FM.mif and imported directly to this document without further alteration. The import command within FrameMaker is under the File option. These plots were produced from the example code.

See Also: FM_1Dm**,** FM_xyPlot**,** FM_scatter**,** FM_histogram

3.4.2 FM_1Dm

Usage:

```
#include <FrameMaker.h>
void FM_1Dm(const char* filename, int N, row_vector* vxs);
```

Description:

The function FM_1Dm creates a FrameMaker file called ***filename*** in MIF format. It will contain plots of the data contained in the ***N*** vectors which are pointed to by ***vxs*** These plot(s) may be further manipulated from within FrameMaker itself. FrameMaker MIF files are typically named with a ".mif" suffix so it is recommended that all filenames used for this function end with .mif.

Return Value:

Nothing. A new disk file in the MIF is produced for incorporation into FrameMaker. It will contain either one or two plots depending on the flag "rc".

Example:

```
#include <gamma.h>
main()
 {
  int i, j, N=5;                              // This many plots
  row_vector vxs[5], vx(101);                 // Blocks for data points
  for(i=0; i<N; i++) vxs[i] = vx;             // Initilize the 5 blocks
  double x;                                   // Working x,y ordinates
  for(i=0; i<101; i++)                        // Fill up data blocks
    {
    x = double(i-50);                         // Offset x (so centered)
    x = x*x/2500;                             // Parabolic function
    for(j=0; j<N; j++)
      vxs[j].put(complex(j*x),i);             // Store this point
    }
  FM_1Dm("FM.mif", N, vxs);                  // Output to FM.mif, N plots
  }
```

FM_1Dm Example Output

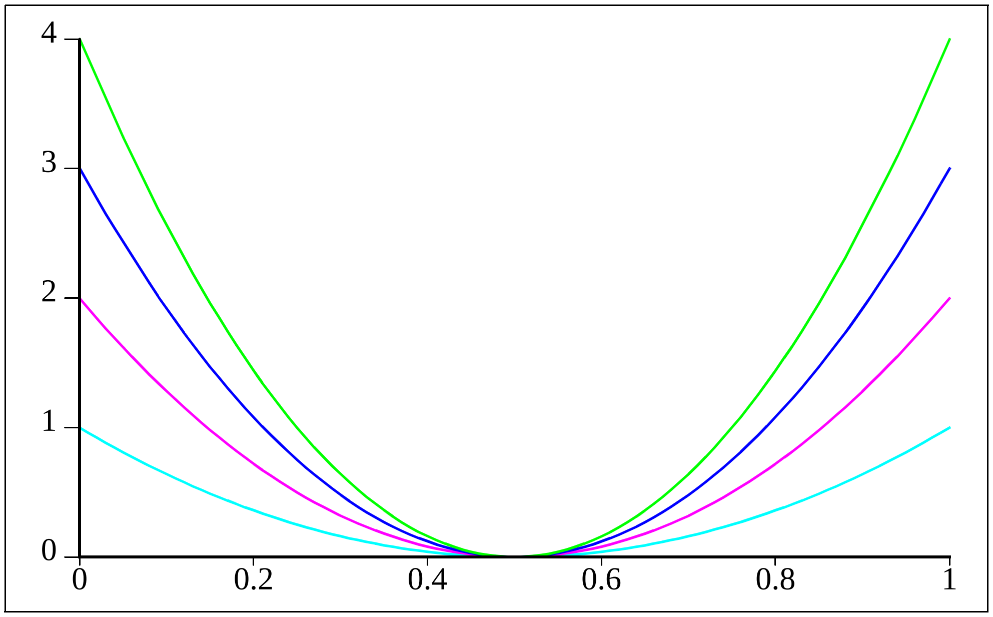


Figure 4-3 - The two plots above were contained in the file FM.mif and imported directly to this document. I did some coloring, resizing, and a bit of axis adjusting in FrameMaker. The import command within FrameMaker is under the File option. These plots were produced from the example code.

See Also: FM_1D, FM_xyPlot**,** FM_scatter**,** FM_histogram

3.4.3 FM_xyPlot

Usage:

```
#include <FrameMaker.h>
void FM_xyPlot (const char* filename, row_vector &vx, double xsize=14, double ysize=14);
```

Description:

The function FM_xyPlot creates a FrameMaker file "filename" in the MIF format. Unlike function FM_1D which assumes the data monotonically increasing on the horizontal axis, FM_xyPlot produces plots in parametric fashion, i.e. true x *versus* y. The plot will be of the data supplied by the vector vx and the plot dimension xsize by ysize in centimeters (default to 14x14 cm plot). It is recommended that "filename" end with ".mif" to signify a FrameMaker MIF file. Note: block_1D can be substituted for row_vector in the function call here.

Return Value:

Nothing. A new disk file is produced for incorporation into FrameMaker.

Example:

```
#include <gamma.h>
main ()
 {
 block_1D BLK(360);                        // create a data block
 double x,y,theta;                         // declare needed variables
 for(int i=0; i<360; i++)                  // loop through 360 degrees
  {                                        // fill up block with Astroid
  theta = i*2.0*PI/360.0;                  // also called a Hypercycloid of four cusps
  x = cos(theta);                          // x = a*[cos(theta)]**3, here a = 1
  y = sin(theta);                          // y = a*[sin(theta)]**3, here a = 1
  x = x*x*x;
  y = y*y*y;
  BLK(i) = complex(x,y);
  }
 FM_xyPlot("astroid.mif", BLK);            // output FrameMaker .mif plot file
 }
```

XY Plot Example

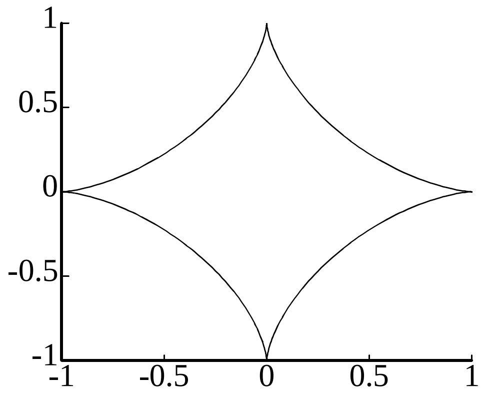


Figure 4-4 - The two plots above were contained in the file FM.mif and imported directly to this document without further alteration. The import command within FrameMaker is under the File option. These plots were produced from the example code.

See Also: FM_1D**,** FM_1Dm**,** FM_scatter**,** FM_histogram

3.4.4 FM_histogram

Usage: ** Note this function works but is still under construction. It may fail if the number of points does not far exceed the number of bins (a factor of >100 seems o.k.)**

```
#include <FrameMaker.h>
void FM_histogram (const char* filename, row_vector &vx, int bins = 0,
                                                        double xsize=14, double ysize=14);
```

Description:

The function FM_histogram creates a FrameMaker file called “filename” in the MIF format The plot will be of the data supplied by the vector vx and the plot dimension xsize by ysize in centimeters (default to 14x14 cm plot). The number of bins is specified by the integer “bins” and should not exceed the number of points in the input data vector. The default number is zero whereupon each point in vx is a separate bin. Currently the data must be increasing monotonic. It is recommended that “filename” end with “.mif” to signify a FrameMaker MIF file. Note: block_1D can be substituted for row_vector in the function call. Each bin of the histogram may be manipulated individually within FrameMaker.

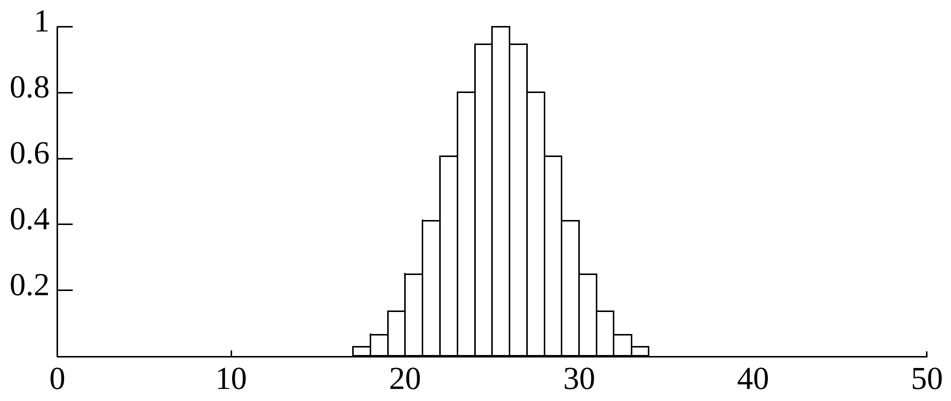
Return Value:

Nothing. A new disk file is produced for incorporation into FrameMaker.

Example:

```
#include <gamma.h>
main ()
 {
 row_vector vx(51);                    // create a data block
 row_vector vx1(51);                   //
 vx1 = Gaussian(51, 25, 3);            // fill up data with Gaussian
 for(int i=0; i<51; i++)
  vx(i) = complex(i, Re(vx1(i)));
 FM_histogram(“FM.mif”, vx, bins); // output FrameMaker .mif plot file
 }
```

Histogram Example



See Also: FM_1D**,** FM_1Dm**,** FM_xyPlot**,** FM_scatter

3.4.5 FM_scatter

Usage:

```
#include <FrameMaker.h>
void FM_scatter (const char* filename, row_vector &vx, int sides=0,
                                        double PGsize=0, double xsize=14, double ysize=14);
void FM_scatter (const char* filename, row_vector &vx, char a='o',
                                                              double xsize=14, double ysize=14);
```

Description:

The function FM_scatter is essentially the same as the function FM_xyPlot except that the points are not connected by a line, they are marked with a specified symbol. The FrameMaker MIF file “filename” is created containing a plot of the data supplied by the vector vx. The plot dimension is xsize by ysize in centimeters (default to 14x14 cm plot). The data is plotted x *versus* y where x are the real points of the vector and y the imaginary points.

1. FM_scatter (const char* filename, row_vector &vx, int sides=0, double PGsize=0, double xsize=14, double ysize=14) - When the function is called with these arguments a graphic object is used to mark the point in the scatter plot. The size of the symbol is given in centimeters by “PGsize” which defaults to 1/100 of xsize. PGsize is the radius of the circle which circumscribes the graphics objects marking the points. The object itself is determined by the value of “sides”. Typically “sides” will be the number of sides of a polygon and defaults to zero in order to indicate a circle. The following are valid numbers for “sides”

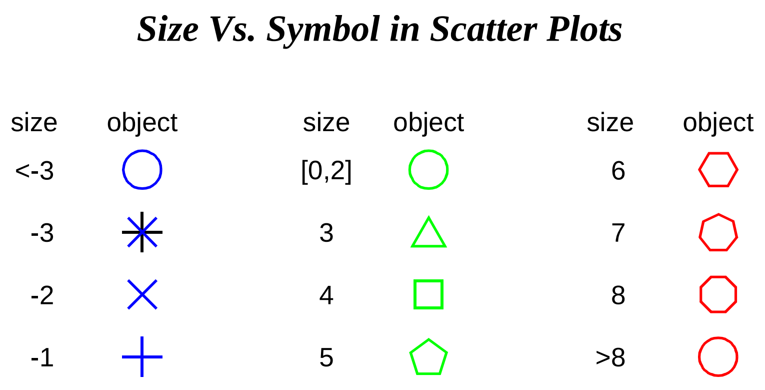


Figure 4-5 - Value of “size” vs. Symbol Output. These may also be set inside FrameMaker..

The objects shown above were taken from plots made with the FM_scatter function using the various size values and 0.25 for PGsize.

2. FM_scatter (const char* filename, row_vector &vx, char a, double xsize=14, double ysize=14) - When the function is called with these arguments it uses a character to mark the points in the scatter plot.

These objects marking the plotted points are grouped together and can be manipulated as a whole or individually inside of FrameMaker. It is recommended that “filename” end with “.mif” to signify a FrameMaker MIF file. Note: block_1D can be substituted for row_vector in this function.

Return Value:

Nothing. A new disk file is produced for incorporation into FrameMaker.

Examples:

```
#include <gamma.h>
main ()
 {
 block_1D BLK(50);                          // create a data block
 double x,y,theta;                          // declare needed variables
 double a,b;                                // declare needed variables
 for(int i=0; i<50; i++)                    // loop through 50 points
  {                                         // fill up block with Prolate Cycloid
  a = 1;
  b = 2;
  theta = -PI + i*(4.0*PI/49.0);            // angles span -pi to 3pi
   x = a*theta - b*sin(theta);              // x = a(theta) - b*sin(theta), here a=1, b=2
  y = a - b*cos(theta);                     // y = a - b*cos(theta)
  BLK(i) = complex(x,y);
  }
 FM_scatter("FM.mif", BLK, 0,.1, 14, 5);    // output FrameMaker .mif plot file
 }
```

FM_scatter Example1 Output

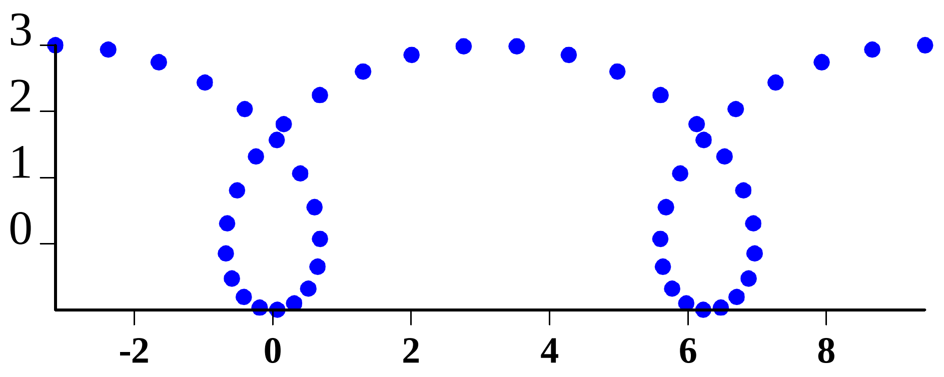


Figure 4-6 - The plot above was contained in the file FM.mif and imported directly to this document. Minor alterations were performed in FrameMaker (coloring, sizing, and axis font changes). The import command within FrameMaker is under the File option. Each symbol can be manipulated individually or all simultaneously within FrameMaker. Thus one can fill the circles, change their sizes, etc. after the plot has been produced. The next example demonstrates this ability and the use of characters to mark the points.

```
#include <gamma.h>
main ()
 {
 block_1D BLK(101);                    // create a data block
 double x,y,a=3;                       // declare needed variables
 for(int i=0; i<51; i++)               // fill block with Strophoid
  {                                    // y**2 = x**2[(a-x)/(a+x)]
  x = (5.5*i/50)-2.5;
  y = sqrt(x*x*(a-x)/(a+x));
  BLK(i) = complex(x,y);
  BLK(100-i) = complex(x,-y);
  }
 FM_scatter("FM.mif", BLK, 'b');       // Output FM scatter plot, letter b marking
 points.
 }
```

FM_scatter Example 2 Output

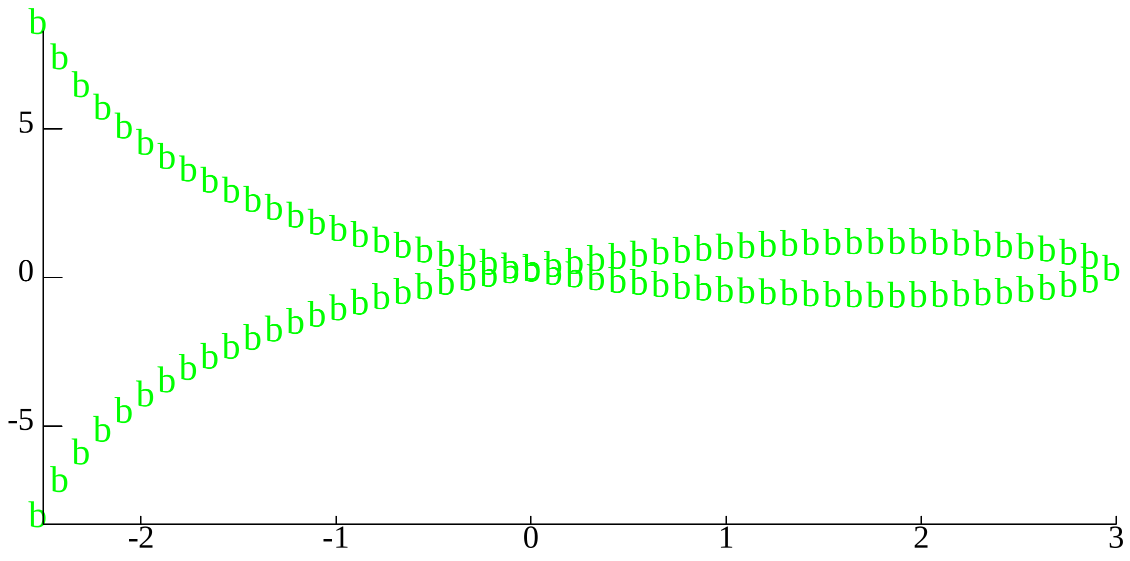


Figure 4-7 This plot above was also produced into a file called FM.mif and imported directly to this document. It has be subsequently altered within Framemaker. First, the overall plot dimensions was changed from the default values of 14cm by 14cm. Second, the plot originally had the character b marking each point. As all points are a single graphics object these b's were all changed simultaneously to a larger font size (default 12pt to 14pt) and to a new font type (Zapfdingbat).

See Also: FM_1D**,** FM_1Dm**,** FM_xyPlot**,** FM_histogram

3.4.6 FM_contour

Usage:

```
#include <FrameMaker.h>
void FM_contour(const char* filename, matrix &mx, double threshold, int steps=3,
                    double CLI=0, double CLM=1, int CPN=1, double xsize=10, double ysize=10);
```

Description:

The functions ***FM_contour*** is used to create contour plots in FrameMaker MIF format.

FM_contour (const char* filename, matrix &mx, double threshold, int steps, double CLI, double CLM, int CPN, double xsize, double ysize) -The function FM_contour creates a FrameMaker file called filename in the MIF format. The produced file will contain a contour plot of the real data contained in the matrix mx. The contours begin at the level set by threshold and increment by the value of CLI. The number of contours is set by steps. The levels increment either geometrically or linearly as set by the value of CLM, the default is linear. Positive and negative contours are set by the flag CPN. For CPN=1 (default), both positive and negative contours are produced. For CPN=0 only the positive contours are output while for CPN=-1 only the negative contours are done. The output file contour plot will be of dimension xsize by ysize (both given in centimeters, default 10 cm).

Contour Parameters -

filename - Although not mandatory, this should be “name.mif” where the .mif indicates a FrameMaker file.

mx - Can be any matrix or block_2D in GAMMA. Note that it is the real data that is contoured.

threshold - This can be a positive or negative quantity. If both positive and negative contours are to be performed, the absolute value will be taken for the first contour of the positives and the negative of the absolute value taken as the first contour of the negative levels. This is shown in the following figure where the dashed line indicates the value of threshold and the arrows indicate the direction of subsequent contour levels.

Choosing Contour Levels

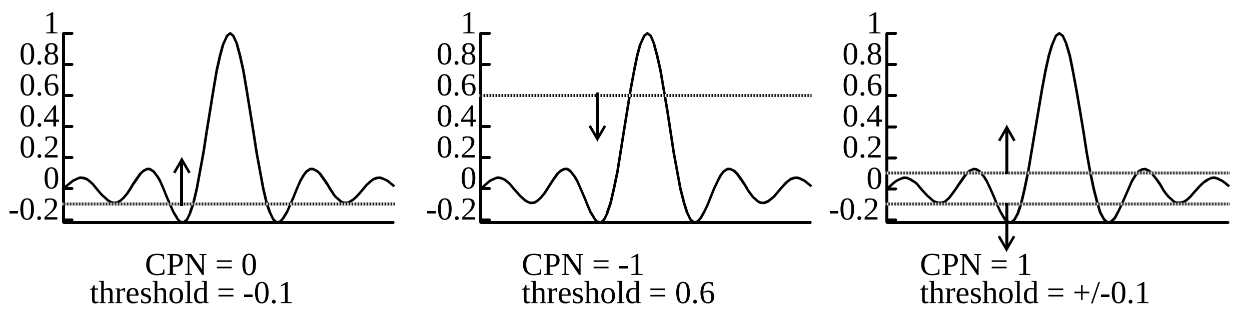


Figure 4-8 - Depiction of the two basic parameters for picking contour levels.

steps - This is the number of contour levels to plot. The default value is 3 and the maximum value is set to 20. If both positive and negative contours are output, there will be still be this number performed in both contour directions. Note that the contours may not be visible in the plot if there is no data in the input matrix corresponding to the contour level.

CLI, CLM - These are the linear and geometric factors which change the contour levels at each step. CLI must have a positive value regardless of whether one desires positive or negative contours. CLM must be positive and >= 1. Typically CLM ranges between 1(default) and 2. The first contour will occur at the value set by threshold (level 0 = threshold). The next contour will be determined strictly by the threshold value and the value of CLI, namely level 1 = threshold + CLI. Subsequent levels are determined jointly by the values of CLM (Contour Level Modifier) and CLI (Contour Level Increment). Generally the contour levels above the initial level 0 are determined from level i = level (i-1) + $[CLI * (CLM)^{i-1}]$. Note that there is a default setting of CLI to zero which flags the contour function(s) to determine an appropriate CLI for the number of steps input. Below are a few 1-dimensional plots depicting how CLM and CLI interact. Setting CPN to -1 would will keep the contour spacing the same but they will decrease in height from the initial level.

Multiple Contour Levels

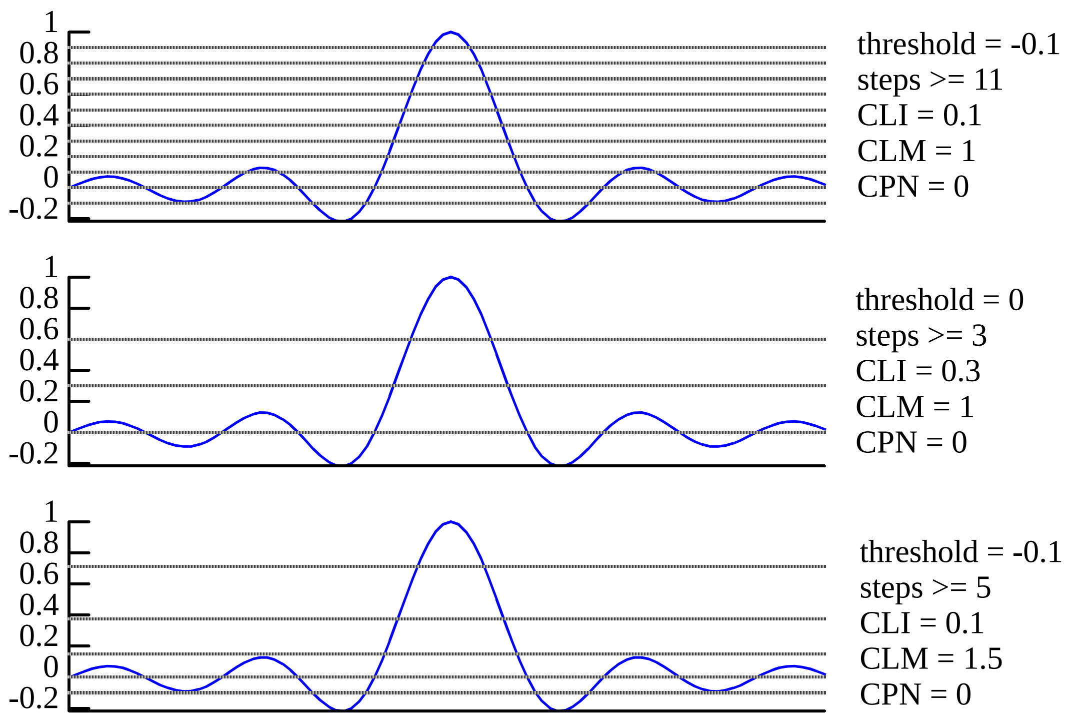


Figure 4-9 - Examples depicting function arguments vs. contour levels chosen..

Setting CPN to 1 will produce the same levels as well as those mirrored vertically about 0, except that the input threshold must be greater than 0. Thus keeping the setting as in the above diagram the but with CPN=1 will force the function to internally alter these input thresholds.

<u>CPN</u> - This is a flag to indicate whether positive (or increasing), negative (or decreasing), or both positive and negative contours. If CPN = 0, only contours increasing from the set threshold will be computed. If CPN = -1 only contours decreasing from the set threshold will be computed. If CPN = 1 (default), contour will be computed increasing from |threshold| and decreasing from -|threshold|.

<u>xsize</u>, <u>ysize</u> - These determine the overall plot dimensions the FrameMaker output will assume. The values are input in centimeters and are defaulted to 10 cm each. The values do nothing to the relative x to y scaling implicit in the data matrix, thus a 256 by 512 array will be 5 x 10 cm even though xsize and ysize are both set

to 10 cm.

Return Value:

Nothing. A new disk file is produced for incorporation into FrameMaker.

Example:

```
#include <gamma.h>
main()
 {
 matrix mx(101, 101);                          // create a 101x101 matrix for data
 row_vector BLK1 = sinc(101, 50, 10);          // use provided window sinc function
 row_vector BLK2 = sin_square(101, 50);        // use provided window sin squared function
 for(int i=0; i<101; i++)                      // loop through and fill up the matrix
  for(int j=0; j<101; j++)
   mx(i,j) = BLK1(i) * BLK2(j);
 FM_contour("contour.mif",mx,.05,10,.05);     //create file FM contour file - contour.mif
 }
```

FM_contour Example Output

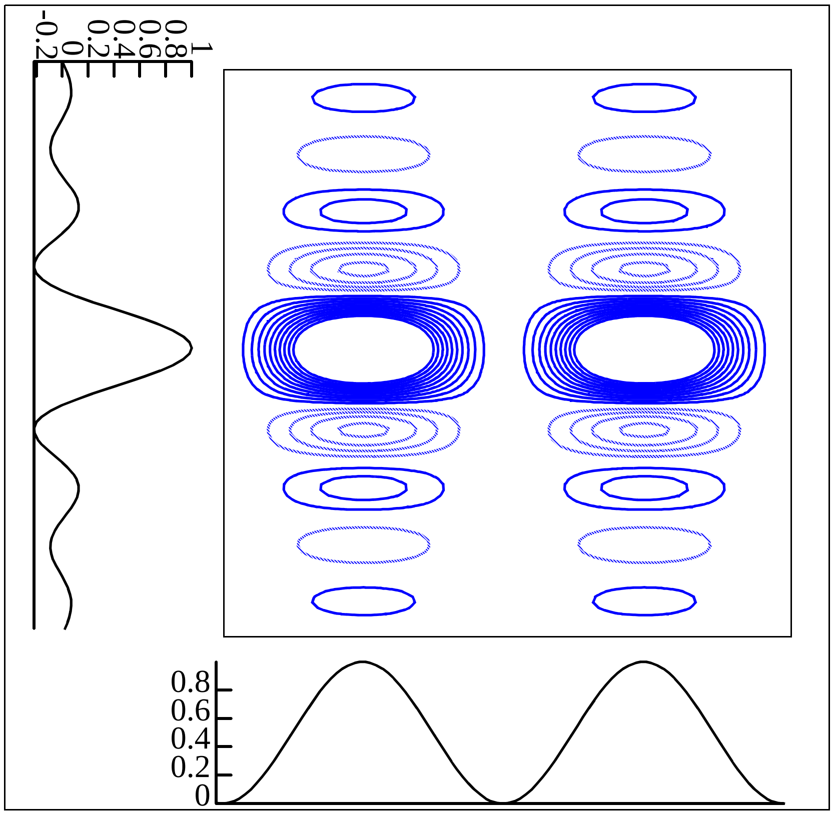


Figure 4-10 Contour plot of the 101x101 matrix which is a $\sin^2(x)$ on one axis and a sinc(y) on the other axis. The first contour is set at +/-0.05 and increments by 0.05 up and down over 10 contours - of which only four of the negative contours exist. The file contour.mif was incorporated directly (contained in the box) to this document using the FrameMaker import command. The plot was resized and the negative contour lines switched to dashed for highlighting. The two 1D-plots were independently generated (with FM_1D) and added for clarity.

See Also: FM_stack

3.4.7 FM_stack

Usage:

```
#include <FrameMaker.h>
void FM_stack(const char* filename, matrix &mx, double xinc, double yinc,
                                   int row_inc, double xsize=14, double ysize=14)
```

Description:

The function FM_stack creates a FrameMaker file called “filename” in the MIF format. It contains a single stack plot of dimension xsize by ysize (both given in centimeters, default 14 cm). The data is input in the form of a matrix and the plot is of the entire matrix real data. The values xinc and yinc, also given in centimeters, are the amount to shift the next row in the horizontal and vertical directions respectively. The rows which are to be plotted are specified by the value row_inc, e.g. a row increment of 3 causes the first, fourth, seventh, etc., until the end of the matrix is reached.

Plotting Parameters - The total plot dimension is specified by the values of xsize and ysize, the entire plot will be scaled to fit into this box. The amount of skewing that the plane containing the baselines, *i.e.* where the zero level of the rows lie, is set by the values of xinc and yinc. This plane is that which is horizontally striped in the figure. The value of Δx is (mxrows+1)*xinc and the value of Δy is (mxrows+1)*yinc where mxrows are the total number of rows in the input matrix. (The 1 is added because there is a border drawn around the plane). Peak intensities will then be scaled to fill the rest of the plot area. Thus, **vertical peak scaling is mainly determined by combination of yinc and ysize**.

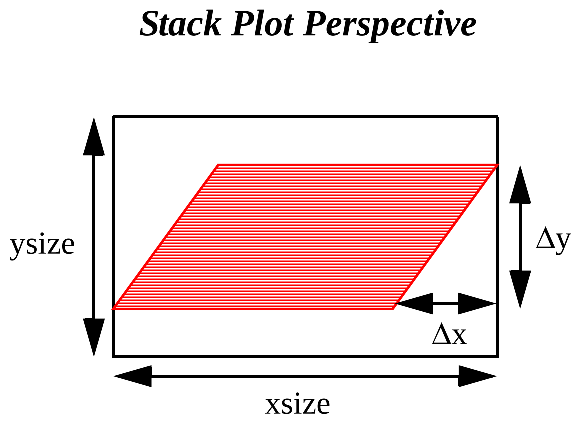


Figure 4-11 - How to set the skew or viewing angle in the FM stack plot function.

Changes made to the row increment, row_inc, somewhat affects plot scaling as well because only the rows actually plotted are considered, not the entire data matrix input. The figure below demonstrates the effect of increasing the value of row_inc.

Stack Plot Row Increments

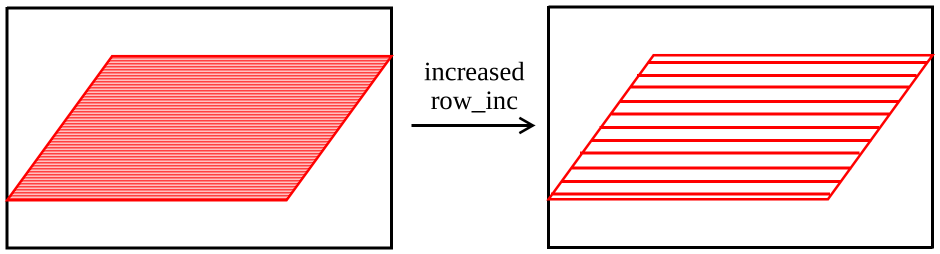


Figure 4-12 - The effect of the row increment arguemnt.

The value of xinc dictates how much horizontal skew there is in the final plot. Negative values are acceptable, this simply changes the orientation as shown in the next figure.

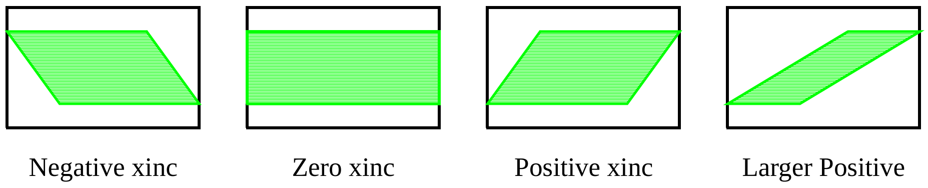


Figure 4-13 - How xinc affects the skewing of the output stack plot.

In a similar fashion, yinc dictates the amount of vertical skew there is. Negative values for yinc are not currently supported and will yield unpredictable plots. Rather it is recommended that the matrix is multiplied by -1 prior to entering this function.

xinc, yinc, and Stack Plots

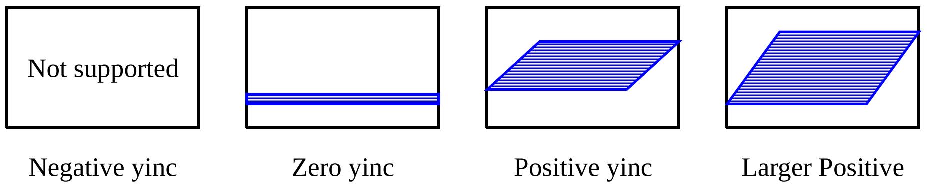


Figure 4-14 - How xinc affects the skewing of the output stack plot.

Graphics Properties - Within FrameMaker, stack plots generated with this function are full graphics objects and have a graphics hierarchy. The entire plot is grouped and can be resized, annotated, or rotated. As a example, the figure below is a stack plot generated with this function which has been manipulated several different ways within FrameMaker.

Graphical Manipulations of Stack Plots Within FrameMaker

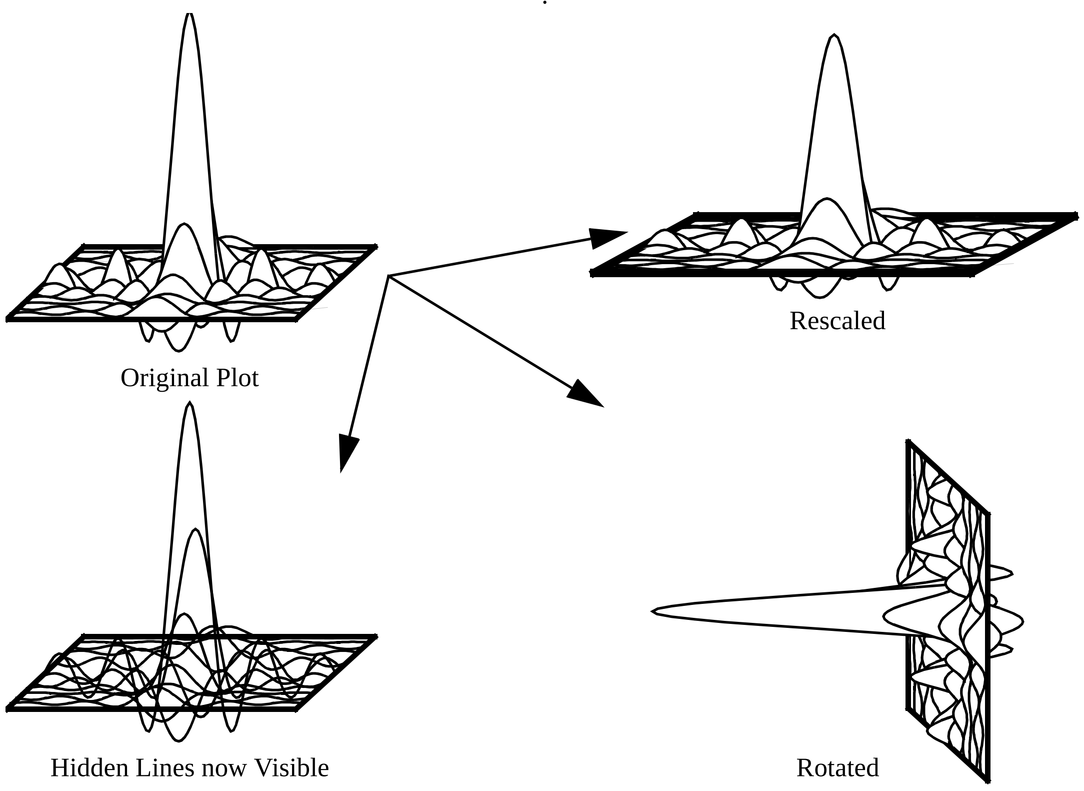


Figure 4-15 - The two plots above were contained in the file FM.mif and imported directly to this document without further alteration. The import command within FrameMaker is under the File option. These plots were produced from the example code.

Furthermore, each row can be individually manipulated also be manipulated as a graphics object as the following diagram illustrates.

More Graphical Manipulations of Stack Plots

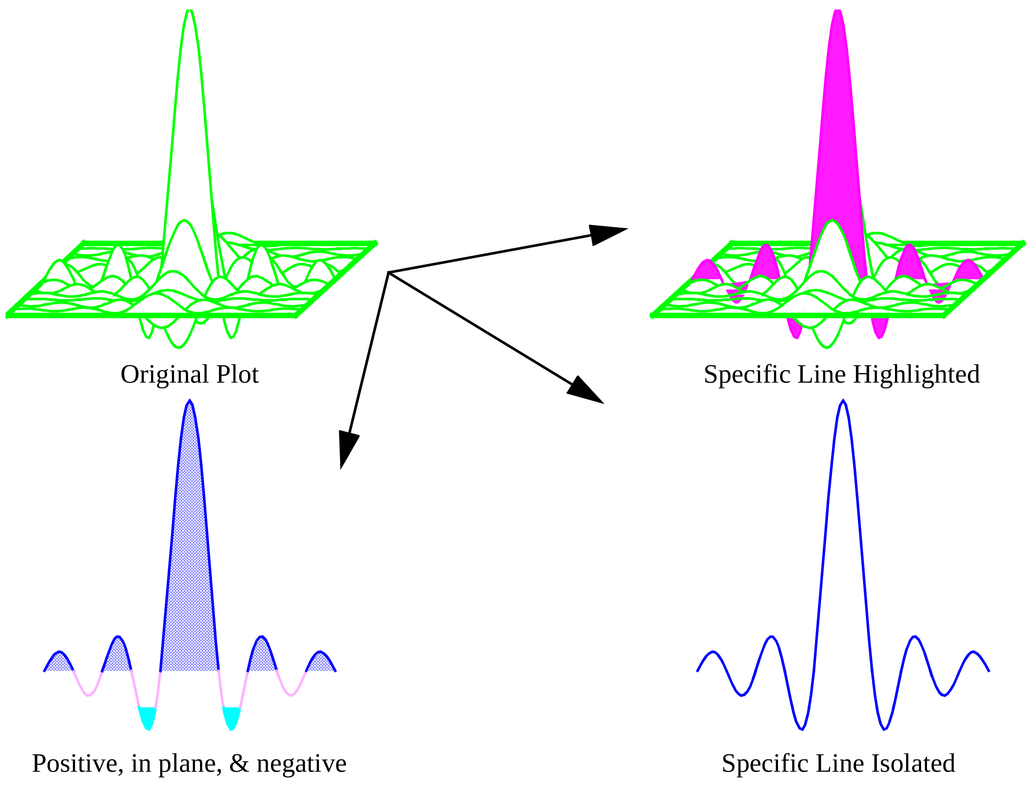


Figure 4-16 - The two plots above were contained in the file FM.mif and imported directly to this document without further alteration. The import command within FrameMaker is under the File option. These plots were produced from the example code.

FrameMaker MIF files are typically named with a ".mif" suffix so it is recommended that all filenames used for this function have a .mif at the end.

Return Value:

Nothing. A new disk file is produced for incorporation into FrameMaker.

Example:

```
#include <gamma.h>
main()
 {
 matrix mx(101, 101);                     // create a 101x101 matrix for data
 block_1D vx(100);                        // create a 1D-data block of length 101
 vx = sinc(101, 50, 10);                  // use provided window sinc function
 for(int i=0; i<101; i++)                 // loop through and fill up the matrix
  for(int j=0; j<101; j++)
   mx(i,j) = vx(i) * vx(j);
 FM_stack("stack.mif", mx, 0.02, 0.02, 1);    // output the FrameMaker .mif plot file
 }
```

FM_stack Example Output

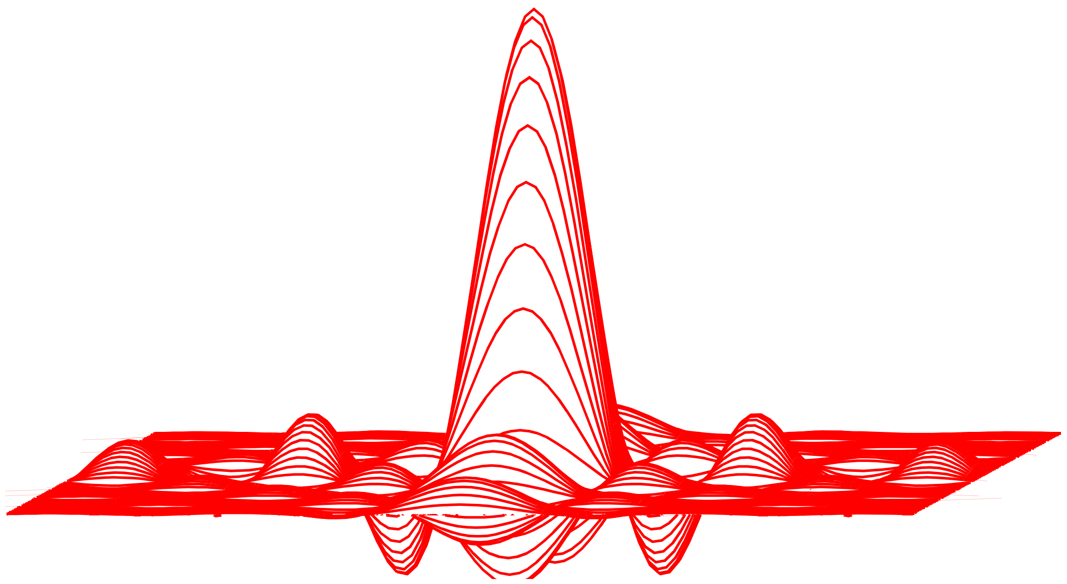


Figure 4-17 This example generates a 101x101 matrix which is a sinc function along both axes. The first contour block plotted is row 0. Each successive row begins 0.02 cm above and 0.02 over from the previous row. In this example the row increment is set to 7. The default dimensions of 14x14 cm are used (because they are left out of the function call). Note that the plot here has been rescaled.

See Also: FM_contour

3.4.8 FM_sphere

Usage:

```
#include <FrameMaker.h>
void FM_sphere(const char* filename, int type=2, double alpha=0, double beta=15,
                                        double gamma=-15, double radius=5, double points=100);
void FM_sphere(const char* filename, coord_vec &data, int type=0, double alpha=0,
                    double beta=15, double gamma=-15, double radius=5, double points=100);
void FM_sphere(const char* filename, coord_vec &data1, coord_vec &data2, int type=0,
 i   double alpha=0, double beta=15, double gamma=-15, double radius=5, double points=100);
```

Description:

The function ***FM_sphere*** creates a FrameMaker file called ***filename*** in the MIF format. It contains a single 3D-plot which has been projected after rotation by the Euler angles ***alpha***, ***beta***, and ***gamma*** (input in degrees) to produce the desired perspective.

1. FM_sphere (const char* filename, int type, double alpha, double beta, double gamma, double radius, int points) - Used in this manner, the function plots no data, only coordinate axes and/or a coordinate sphere depending on the value of type. For type = 0, the three coordinate axes are drawn of (unprojected) length 2*radius. For type=0, the coordinate sphere having radius of radius is drawn along with it's intersection with the three planes (xy, xz, & yz). For type = 2, both the axes and the sphere are drawn. The value of points specifies how many points to use when drawing each sphere-plane intersection.
2. FM_sphere (const char* filename, double coord_vec, int type, double alpha, double beta, double gamma, double radius, int points) - When the function is called with these arguments it draws the plot produced in the description above (1.) with both axes and the coordinate sphere. It then adds the data contained in the coord_vec data to the plot.
3. FM_sphere (const char* filename, double coord_vec, double coord_vec, int type, double alpha, double beta, double gamma, double radius, int points) - When the function is called with these arguments is the same as the previous description (2.) but plots both data sets, data1 and data2.

2D Projection - Initially, the coordinates and/or drawn coordinate system is rotated by the specified Euler angles. The rotated three dimensional coordinates are then projected onto the 2D plane of the paper (or screen). To produce a reasonable plot the 3D z-coordinates is mapped into the 2D y-coordinates and the 3D x-coordinates are mapped into the 2D negative x-coordinate as depicted in the figure below. This mapping keeps everything related to standard right-handed coordinate systems. The initial, unrotated system has y coming up out of the paper plane.

Figure 4-18 - Depiction of (simple) 3D Euler Rotation and subsequent projection on plot axes.

Perspective, Euler Rotations - The three Euler angles can dramatically change the quality of the out put plot. The default Euler angles are set to produce a nice view of typical data, maintaining the z axis vertical. The following figures demonstrate by example the effect of the various Euler angles on the final coordinate axes in which the data is drawn.

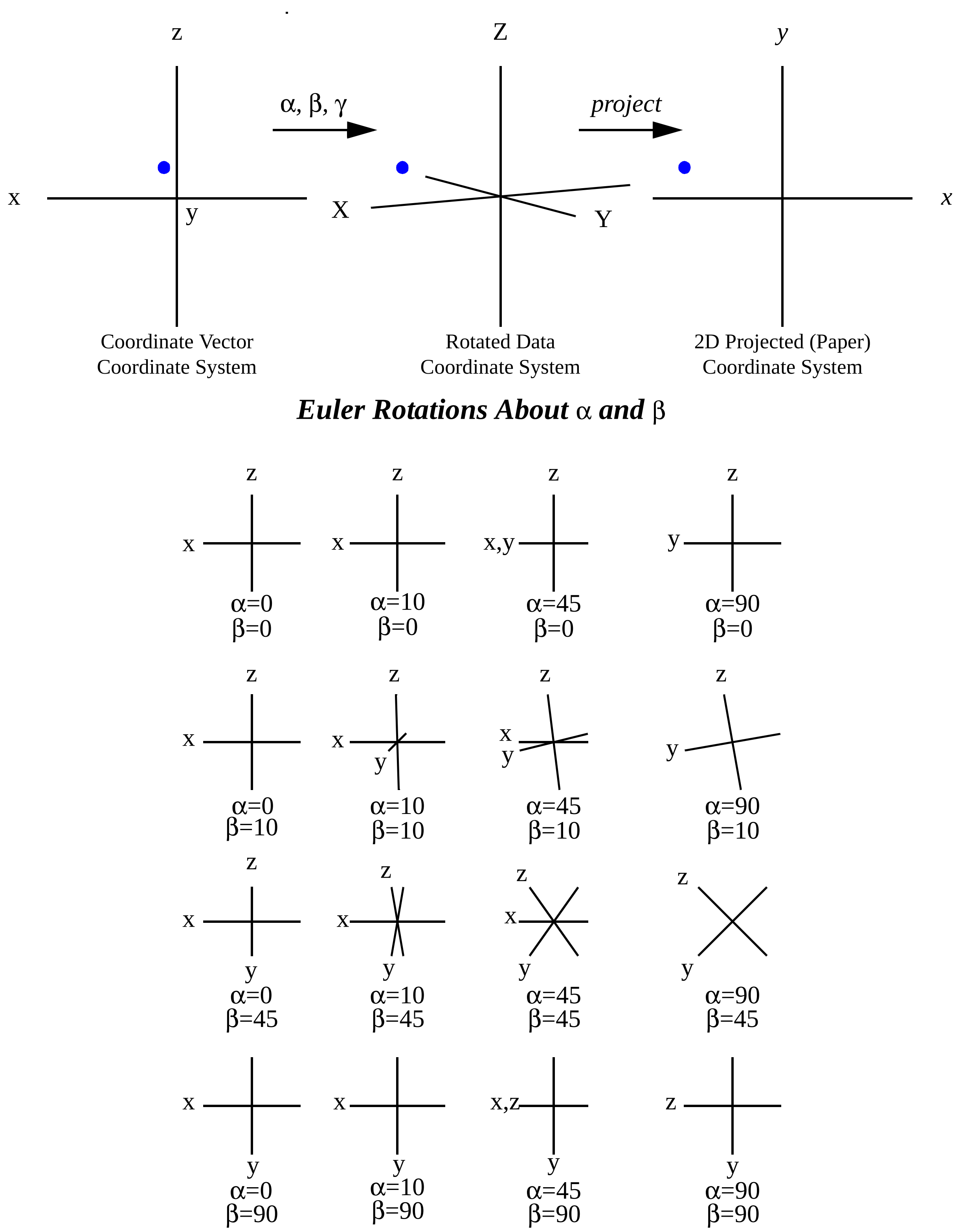


Figure 4-19 - Examples of rotations using only the 1st two Euler Angles.

These axes were generated with the program listed as Example 1 using a radius of 1 (cm), a gamma value of zero (degrees), and type 0 (only axes). The axis orientation proceeds via first rotating about the z axis with angle alpha followed by rotation about the new x axis with angle beta. The last rotation, if gamma were non-zero, is about the new z axis with angle gamma. Looking from the positive axis toward the origin, all rotations appear clock-wise[1].

Euler Rotations About β ***and*** γ

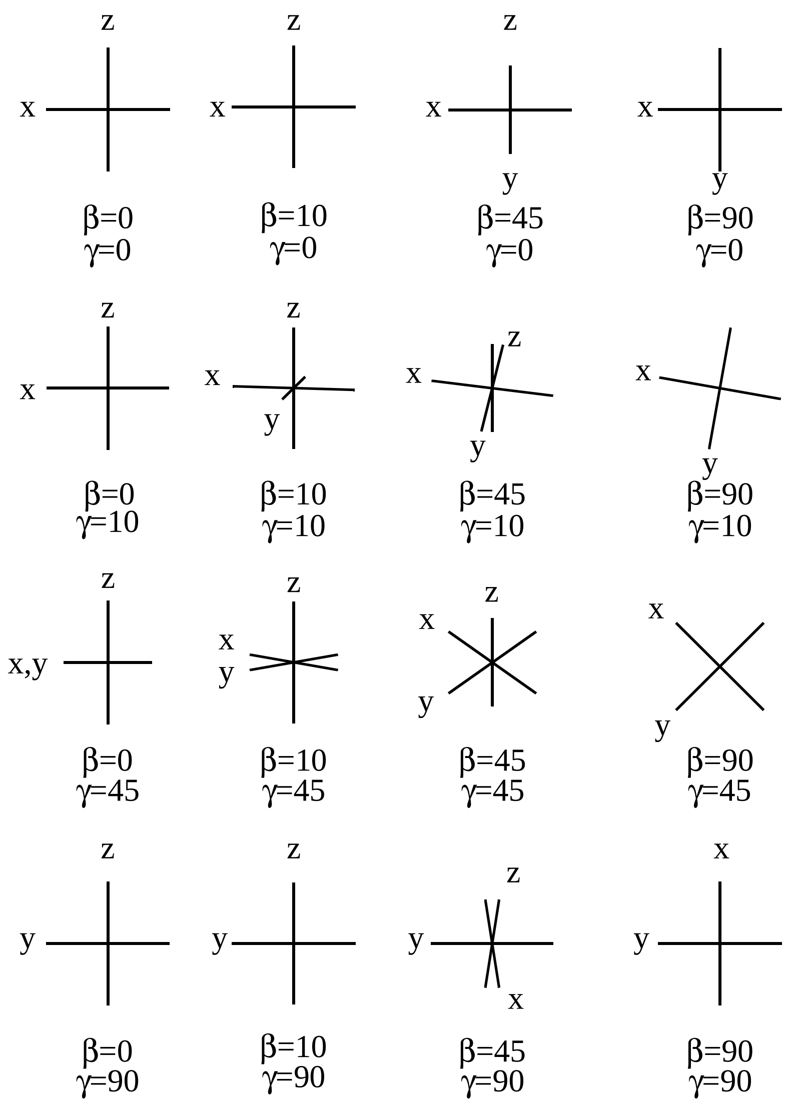


Figure 4-20 Again, these axes were generated with the program listed as Example 1. The axis ori-

1. Euler rotations follow the right hand rule, that is, the coordinate system moves counter-clockwise about the rotation axes. An alternate and equivalent view is that the coordinates themselves move clock-wise about stationary axes. This function strictly adheres to this convention. The overall plot is reference to some static axes. Any data is thus rotates by input Euler angles clock-wise relative to these stationary axes. The axes sketched by this function are axes for the data (absent in one function usage) of the input coordinate vector, not the overall static reference axis. Thus, the rotations of the plotted axes follow the rotation convention of the coordinates themselves: they rotate clockwise about the axes of rotation.

entation proceeds via first rotating about the z axis with angle alpha (in this case alpha=0, so not performed), followed by rotation about the new x axis with angle beta (in this case about the original x-axis), and then followed by rotation about the new z axis with angle gamma.Looking from the positive axis toward the origin, all rotations appear clock-wise.

Example 1:

```
#include <gamma.h>
main ()
 {
 cout << “\nPlease input a radius(cm): “;
 double radius;
 cin >> radius;
 cout << “\nPlease input a Euler angle alpha(deg): “;
 double alpha;
 cin >> alpha;
 cout << “\nPlease input a Euler angle beta(deg): “;
 double beta;
 cin >> beta;
 cout << “\nPlease input a Euler angle gamma(deg): “;
 double gamma;
 cin >> gamma;
 cout << “\nPlease input plot type (0=axes, 1=planes, 2=both): “;
 int type;
 cin >> type;
 FM_sphere(“FM_sph1.mif”, type, alpha, beta, gamma, radius);
 }
```

FM_sphere Example 1 Output

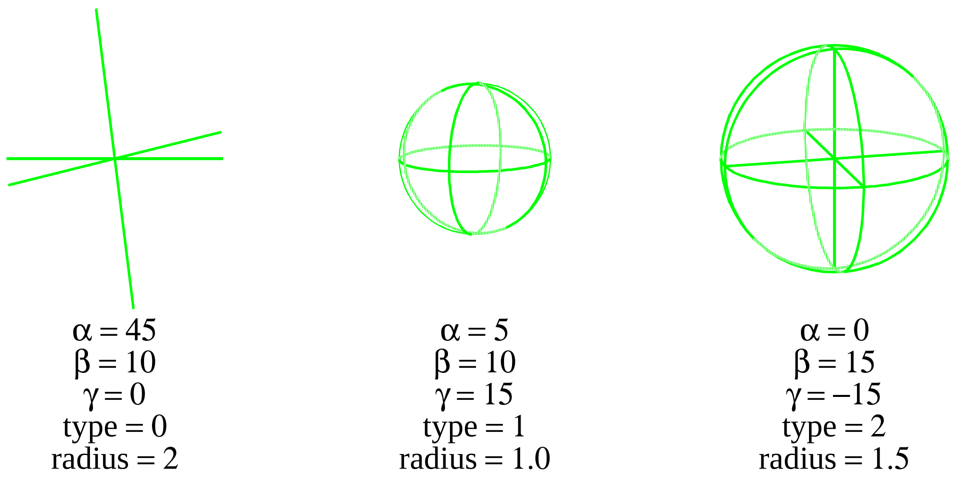


Figure 4-21 This example program runs interactively and prompts the user for information concerning the plot. Here, the function FM_sphere is used only to produce a coordinates system plot - either axes, the coordinates sphere, or both.

Example 2:

```
#include <gamma.h>
main ()
 {
 coord_vec data1(500);                        // Declare a 500 point coordinate vector
 coord_vec data2(500);                        // A second coordinate vector
 double xx, yy, zz;                           // Declare needed variables
 double theta;                                // Declare an angle variable
 for(int i=0; i<500; i++)                     // Fill data1 with a spiral
  {
  theta = i*6.0*PI/499.0;
  xx = 3.0*cos(theta);
  yy = 3.0*sin(theta);
  zz = 3.0 - (6.*i/499.);
  data1.put(xx, yy, zz, i);
  }
 data2 = data1.rotate(90,90,0);               // Set 2nd coordinate vector to rotated data1
 FM_sphere("FM_sph2a.mif", data1,0);          // Output FrameMaker file FM_sph2a.mif
 FM_sphere("FM_sph2b.mif", data2,1);          // Output FrameMaker file FM_sph2b.mif
 }
```

FM_sphere Example 2 Output

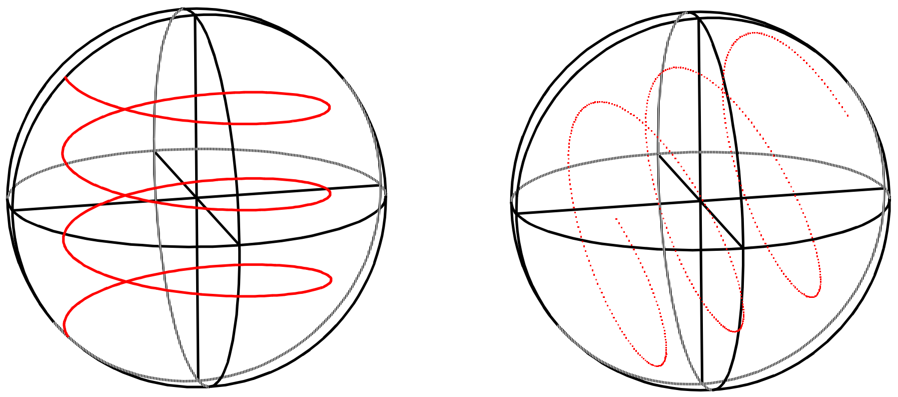


Figure 4-22 This example demonstrates the use of the function FM_sphere for plotting a coordinate vector. The value of <u>type</u> indicates whether the plotted data should be a solid line, individual points, or vectors (see Example 3). The function rotate is a member function of a coordinate vector. The sphere size (default 5 cm radius) was altered to 2.5 cm radius within FrameMaker.

Example 3:

```
#include <gamma.h>
main ()
 {
  int size = 31;                          // Set 31 points
  coord_vec traj1(size);                  // Declare two coordinate vectors
  coord_vec traj2(size);
  double xx, yy, theta;
  for(int i=0; i<size; i++)               // Fill coordinate vectors
   {                                      // Trajectory 1 is in the yz plane
   theta = (PI/2.0)*i/(size-1);           // decreasing from (001) to (010)
   xx = cos(theta);                       // Trajectory 2 is in the xz plane
   yy = sin(theta);                       // decreasing from (100) to (00-1)
   traj1.put(0,yy,xx,i);
   traj2.put(xx,0,-yy,i);
   }
  FM_sphere("FM_sph2.mif", traj1,         // Output FrameMaker MIF file
              traj2, 2, 0.0, 15.0, -45.0); // Euler angles for nice perspective
 }
```

FM_sphere Example 3 Output

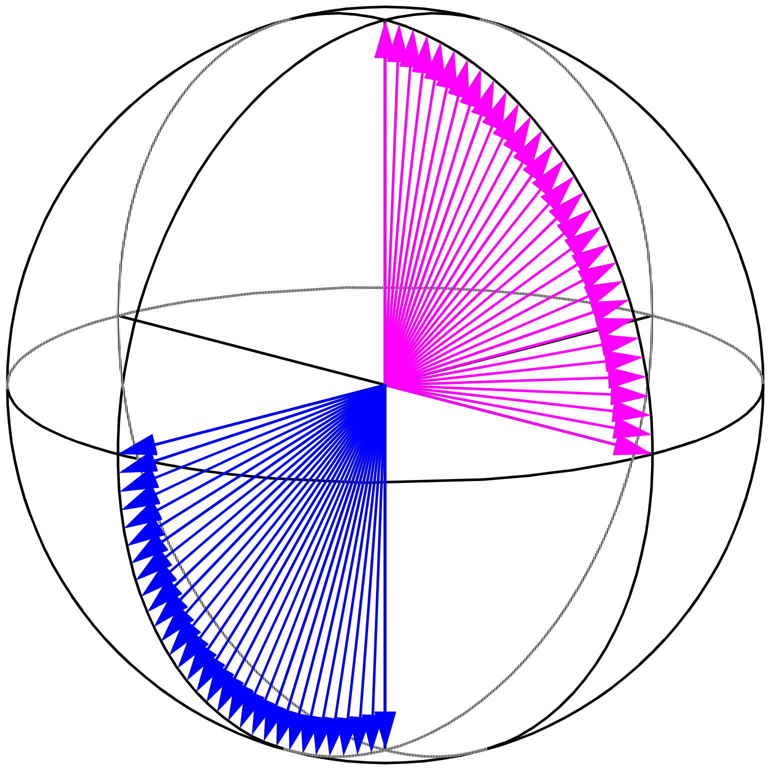


Figure 4-23 - The two plots above were contained in the file FM.mif and imported directly

to this document without further alteration. The import command within FrameMaker is under the File option. These plots were produced from the example code.

See Also: None

3.5 Routines for Matrix Output in FM

3.5.1 FM_Matrix

Usage:

```
#include <FrameMaker.h>
void FM_Matrix (const char* filename, gen_op& Op, int prec = 2, int threshold = 0.001);
void FM_Matrix (const char* filename, matrix& mx, int prec = 2, int threshold = 0.001);
```

Description:

The function ***FM_Matrix*** generates a FrameMaker Mathematical Language (MML) file which can be directly imported into a FrameMaker Document. For floating numbers, prec (default=2) digits after the decimal point will be used. If either the real or imaginary part has a norm of lower than threshold, it will be left away on output. If both, the real and imaginary part are below threshold, a simple 0 is written to Output.
If a floating number is closer then threshold to the nearest integer, the integer is outputed.(See example below).

Return Value:

Nothing. A new disk file in the MMF is produced for incorporation into FrameMaker.

Example:

```
#include “gamma.h”
main()
 {

 matrix c;
 cin >> c;
 cout << c;
 FM_Matrix (“Testa1.mmf”,c);
 }
```

Dialog From Program Execution:

```
>3 3
>1.0 0.0
>1.001 0.0001
>0 0.00001
>0 .1
.>1 0
>5 3.00001
>4 4
>5 5
>6 6
3 x 3 full matrix
```

```
( 1.00, 0.00) ( 1.00, 0.00) ( 0.00, 0.00)
( 0.00, 0.10) ( 0.10, 0.00) ( 5.00, 3.00)
( 4.00, 4.00) ( 5.00, 5.00) ( 6.00, 6.00)
```

Testa1.mmf file imported directly into this document:

$$\begin{bmatrix} 1 & 1.00 & 0 \\ 0.10 \cdot i & 0.10 & (5 + 3 \cdot i) \\ (4 + 4 \cdot i) & (5 + 5 \cdot i) & (6 + 6 \cdot i) \end{bmatrix}$$

Figure 4-24 - The two plots above were contained in the file FM.mif and imported directly to this document without further alteration. The import command within FrameMaker is under the File option. These plots were produced from the example code.

Note that the 1,1 is set to the integer 1, the 1,2 element to 1.00 because its full value is 1.001. The imaginary part has a value of 0.0001 and falls below threshold.

See Also: FM_Mat_Plot

3.5.2 FM_Mat_Plot

Usage:

```
#include <FrameMaker.h>
void FM_Mat_Plot (const char* filename, gen_op& Op, int threshold = 0.001);
void FM_Mat_Plot (const char* filename, matrix& mx, int threshold = 0.001);
void FM_Mat_Plot (const char* filename, gen_op& Op, gen_op& ref_Op, int threshold = 0.001);
void FM_Mat_Plot (const char* filename, matrix& mx, matrix& ref_mx, int threshold = 0.001);
```

Description:

The function FM_Matrix generates a FrameMaker Interchange Format (MIF) file which can be directly imported into a FrameMaker Document. The file contains a graphical depiction of the matrix or the operator. Whenever the norm of an element is larger then threshold, a black square is put to the appropriate position. For the forms with two Operator or Matrices on input, black squares are placed everywhere where the difference in the norm of the elements of the two respective matrices is above threshold.

Return Value:

Nothing. A new disk file in the MIF format is produced for incorporation into FrameMaker.

Example:

```
#include “gamma.h”
main()
 {

 matrix c;
 cin >> c;
 cout << c;
 FM_Mat_Plot (“Testa1.mif”,c,1.0);
 }
```

Dialog of Program Execution:

```
>3 3
>1.0 0.0
>1.001 0.0001
>0 0.00001
>0 .1
.>1 0
>5 3.00001
>4 4
>5 5
>6 6
3 x 3 full matrix
( 1.00, 0.00) ( 1.00, 0.00) ( 0.00, 0.00)
( 0.00, 0.10) ( 0.10, 0.00) ( 5.00, 3.00)
```

(4.00, 4.00) (5.00, 5.00) (6.00, 6.00)

Testa1.mif file imported directly into this document:

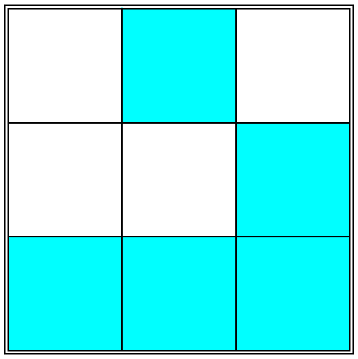


Figure 4-25 - The result of the example program read into this document.

See Also: FM_Matrix

3.6 Mathematical Details & Code Specifics

3.6.1 FrameMaker Contour Plots

The contouring function takes a GAMMA matrix and slices through specified contours to produce a FrameMaker MIF output file. An attempt is made to group all points for each specific contour line together as a single PolyLine. Following this, all PolyLines for a specific contour level are grouped together. As a last step, all positive contours are grouped together as are all negative contours. The contouring algorithm processes the matrix in the following general order.

- I Function arguments are checked for validity and adjusted if necessary (***contour_setup***).
- I Any positive or increasing contours are first taken followed by any negative contours.
- I Individual contours are converted to FM PolyLines in the function ***contour_level***.
- I Contours are grouped together as all positives and/or all negatives in ***group_contours***.

I Initially, the function ***FM_contour*** checks its input arguments with the auxiliary function ***contour_setup***. This function first checks that the overall plot size is reasonable: $xsize \ni [5cm, \mathbf{20}cm]$ & $ysize \ni [5cm, 27cm]$. Then it insures that the input matrix is large enough to be contoured, the smallest allowed matrix is 5x5. A scaling factor for cm/point is then computed, this is the same in both dimensions to keep the relative contour plot size proper in the two dimensions. The next check looks for the matrix global maximum and minimum. If these are the same the matrix will contain no contours and the function signals an error. A check is also made to insure that the number of contours requested is reasonable: $\boldsymbol{steps} \ni [\mathbf{1}, \mathbf{20}]$. Then, the input value of CPN (sets how contouring is done) is checked: $CPN \ni [\mathbf{1}, 0, -1]$. Based on the requested contours, the input threshold (initial contour) is checked to insure that some contours will exist.

I At this point, the function ***FM_contour*** begins looping through the chosen contour levels. Looping through positive (or increasing) contours is first performed if ***CPN >= 0***, then looping is done for negative (or decreasing) contours if ***CPN != 0***. When taking positive (or increasing) contours, searching begins at the value ***threshold***. Negative (or decreasing) contours start at either ***+/-threshold*** depending upon whether positive contours have be taken.

Contours

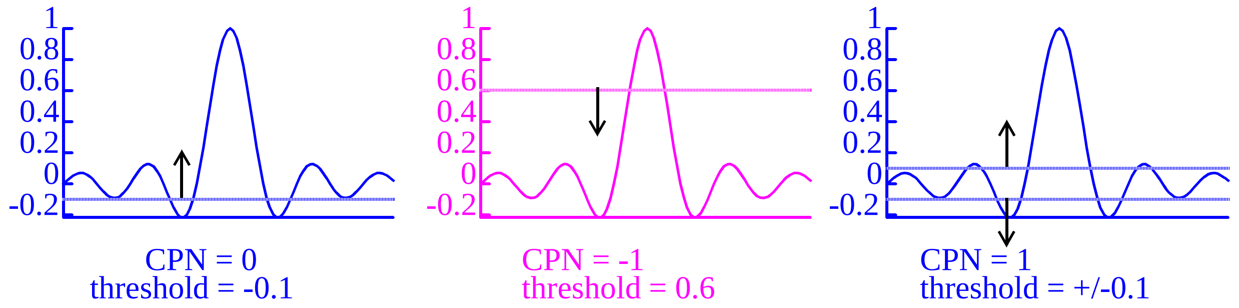


Figure 4-26 - The two plots above were contained in the file FM.mif and imported directly to this document without further alteration. The import command within FrameMaker is under the File option. These plots were produced from the example code.

Before the contour looping begins, the value of ***CLI*** is set so that successive contour levels are either larger (+ or increasing contours) or smaller (- or decreasing contours). Additionally, the value of ***extremum*** is set to the maximum or minimum contour level. If contouring is set in the function call to go beyond the matrix maximum/minimum the value of ***extremum*** will stop unnecessary contouring. Thus, contouring for positives or negatives will stop if ***abs(threshold) > abs(extremum)***.

As looping begins over the number of contours desired, ***steps***, the contour number is set to ***level***, the contour value is set to ***acthresh***, and the contour ID ***conID*** is set[1]. Actual contouring on an individual level is performed is the auxiliary function ***contour_level***. When contouring is completed for a value of ***acthresh*** the value is adjusted and the loop continues to the next contour level. The contour levels are set to change either monotonically or geometrically depending upon the value of ***CLM***.

$$acthresh_{level} = acthresh_{level-1} + [CLI \times CLM^{level-1}]$$

When ***CLM=1*** the levels will change monatomically and when ***CLM>1*** the levels change in geometric fashion[2].

1. The contour ID is set for use in FrameMaker. Each contour is given an individual ID so that it is a specific graphic object within FrameMaker. Subsequently, each contour may be independently manipulated within FrameMaker.
2. Values where ***CLM<0*** are disallowed. If the function is called with ***CLM<0*** it is replaces by ***CLM=abs(CLM)*** in the function ***contour_setup***.

Multiple Contours

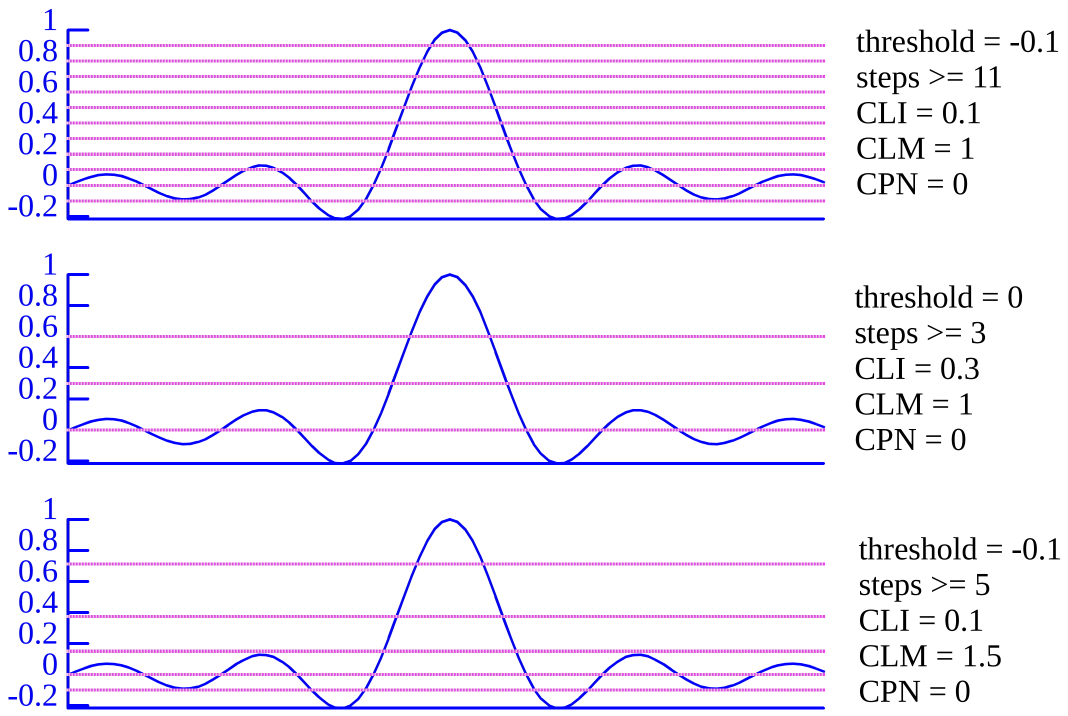


Figure 4-27 - The two plots above were contained in the file FM.mif and imported directly to this document without further alteration. The import command within FrameMaker is under the File option. These plots were produced from the example code.

I Contouring for an individual level is performed in the routine ***contour_level***. In this function the entire matrix is scanned for possible contours and these are (hopefully) converted into FrameMaker PolyLines. The algorithm used is based on a three point search of all the data in the matrix. Looping occurs over all matrix points[1] ("horizontally" as the column index changes more rapidly than the row index), $P_1 = \langle i|mx|j\rangle$. For each P_1, a second point P_2 is chosen which is the first diagonal relative to P_1, namely $P_2 = \langle i+1|mx|j+1\rangle$. These two points form the corners 2x2 sub-matrix, and a triangle is formed with a third point of this sub-matrix; first an upper triangle with point $U = \langle i|mx|j+1\rangle$, then a lower triangle with point $L = \langle i+1|mx|j\rangle$.

1. The points in the last matrix row and column are never chosen as the point P_1 but are included in the contouring as they will be taken as either P_2, U, or L eventually.

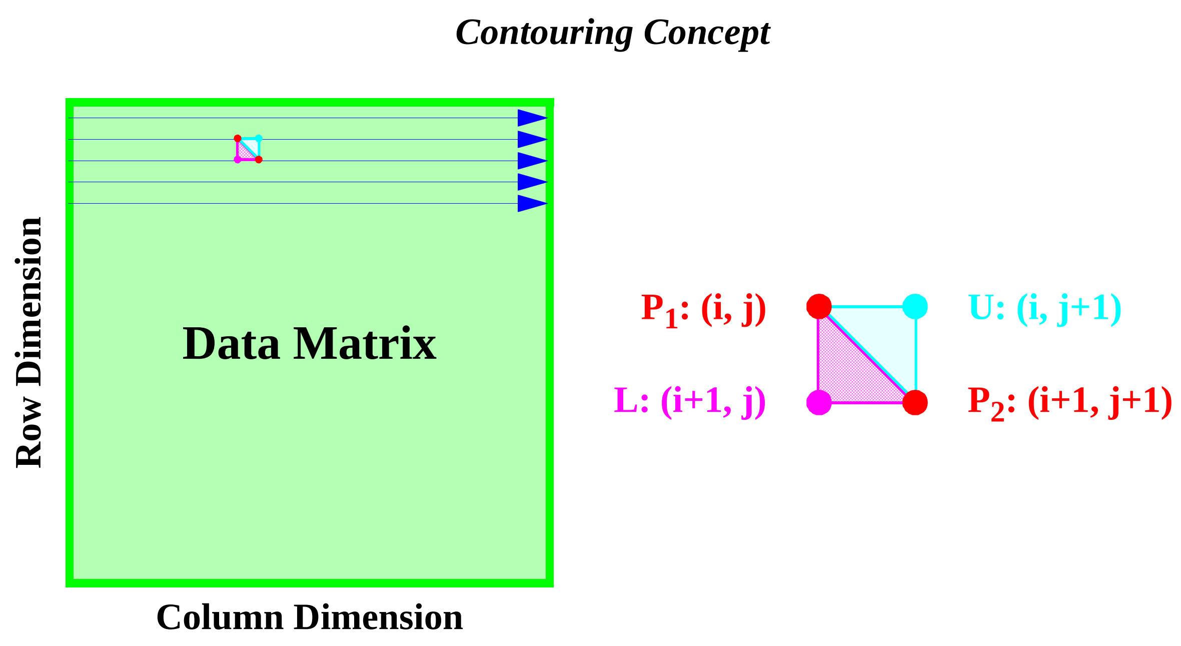


Figure 4-28 - How a matrix is searched for contours in the GAMMA FM_contour function.

For each triangle formed, both upper and lower, function ***contour_level*** determines whether a contour line passes through it and if so the two points where the contour line intersects the triangle there are eight unique situations which exist in looking for a contour line in the triangle, as given in the following table.

Table 1: Eight (2^3) Triangle Based Contouring Situations Possible

1st Point (2^2)	2nd Point (2^1)	3rd Point (2^0)	Situation
P_1 >= threshold (0)	P_2 >= threshold (0)	U/L >= threshold (0)	0
P_1 >= threshold (0)	P_2 >= threshold (0)	U/L< threshold (1)	1
P_1 >= threshold (0)	P_2 < threshold (2)	U/L >= threshold (0)	2
P_1 >= threshold (0)	P_2 < threshold (2)	U/L< threshold (1)	3
P_1 < threshold (4)	P_2 >= threshold (0)	U/L >= threshold (0)	4
P_1 < threshold (4)	P_2 >= threshold (0)	U/L< threshold (1)	5
P_1 < threshold (4)	P_2 < threshold (2)	U/L >= threshold (0)	6
P_1 < threshold (4)	P_2 < threshold (2)	U/L< threshold (1)	7

Based on the binary T/F conditions for each point of the triangle, there are 8 situations possible, one of which will occur for each specific triangle. These can be visualized, as shown in the following figure (upper triangle shown only). Two of these, #0 - all points above the contour level, and #7 - all points below the contour level will contain no contour contribution. All the other situations will contribute to some contour on the contour level being examined. The contour line contributions are shown in thick solid lines. By using a linear fit, the endpoints of the solid lines (where the triangle intersects the contour plane) are calculated in routine ***contour_level*** and forwarded to the function ***PL_contour*** which decides how they contribute to the contour.

Contouring Theme

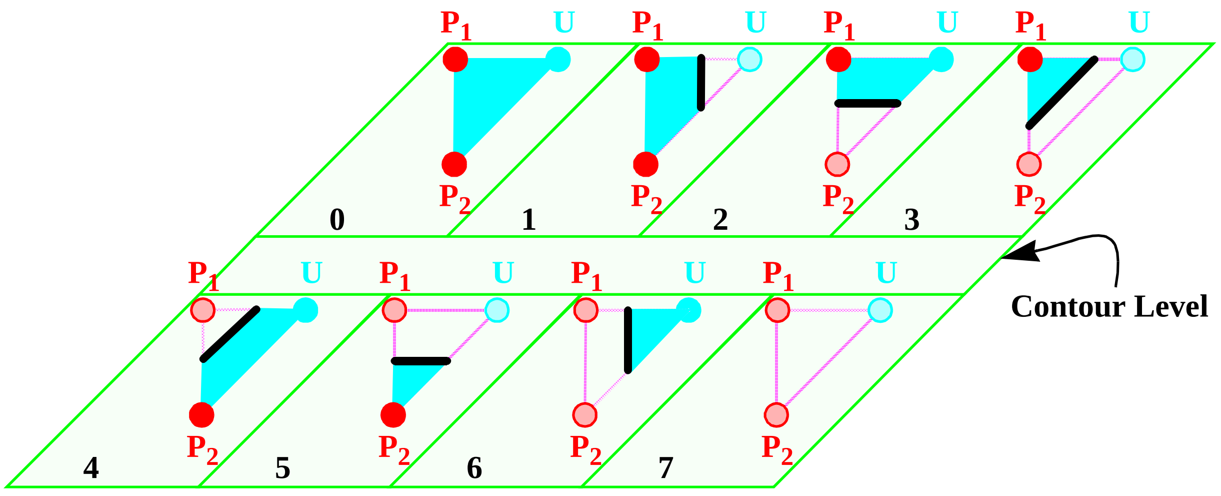


Figure 4-29 - Possible interasections between 3 points and a contour plane.

The diagrams in the previous figure are a bit contrived because the points are rendered to show the matrix i,j (or x,y) spacing and do not exhibit the point intensities (or z). Thus the lines crossing the plane appear vertical, horizontal, or parallel with the skew of the plane itself. This is not the case for the matrix points which actually form these triangles whose z-values will likely vary. Again, for each upper and lower triangle either two or zero points are thus generated which belong to some contour line in the contour level being treated. These two points are passed on to the function ***PL_contour*** which places them into a FrameMaker Polyline.

These two contour points occur where two of the three triangle lines $\{P_1-U, P_1-P_2, U-P_2\}$ cross the contour level plane (or $\{P_1-L, P_1-P_2, L-P_2\}$ for the lower triangles), so determining their values is accomplished by solving the problem of where a line in 3-dimensional space crosses a plane[1]. Using vector notation, a plane is defined by the scalar product relationship which exists between a vector in the plane and a vector normal to the plane. For the contour level plane this would be then

$$\vec{P}_{plane} \bullet \vec{k} = 0$$

where $\vec{P}_{plane}$ is the arbitrary vector which lies in the contour plane and $\vec{k}$ a (unit) vector along the z-axis and perpendicular to the contour plane[2]. Since the contour level plane lies horizontal, the

1. The solution is taken from “Mathematics for Chemists”, Charles L. Perrin, Wiley-Interscience, John Wiley & Sons, Inc., New York, 1970. See page 181 of that text.

vector $\vec{P}_{plane}$ can be taken as the difference of a vector $(threshold)\vec{k}$ with the intersection point vector desired.

$$\vec{P}_{plane} = \vec{P}_{intersect} - (threshold)\vec{k}$$

The first vector may be thought of as one which starts at the origin, runs along the z-axis and is of length $threshold$, whereas the second can be assumed as starting at the origin and ending at the intersection point. One of the two $\vec{P}_{plane}$ vectors for triangle situation 2 is shown in the next figure.

Contouring Situation

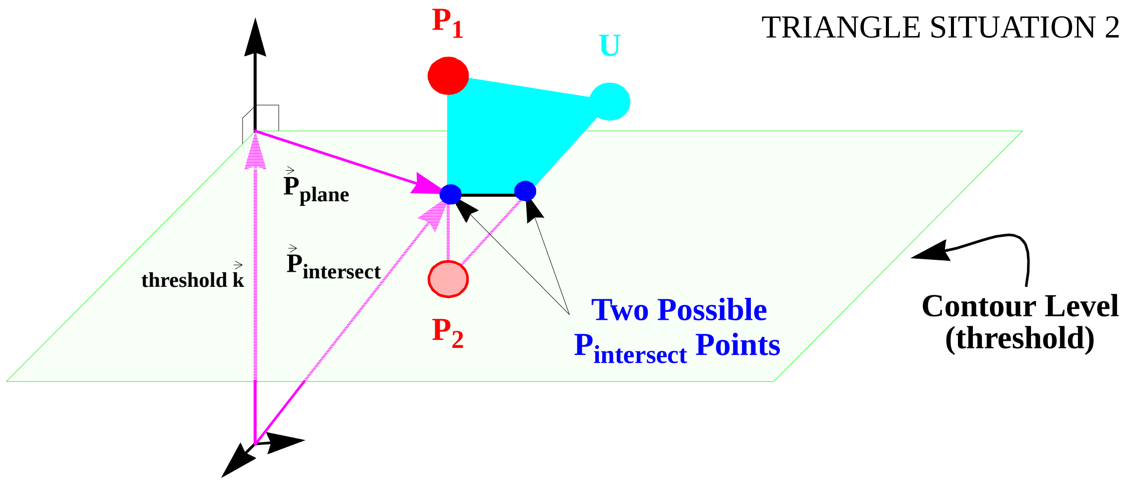


Figure 4-30 - First type of intersection with a contour plane.

As for the 3-dimensional line, $\vec{T}$, which intersects the contour plane we may choose any scalar multiple of the triangle edges which pass through the plane. Which (if any) triangle edges to choose will also depend upon which of the eight situations is under consideration. Expanding upon the previous figure, one of the two possible lines $\vec{T}$ is shown.

2. When use the normal vector as $\vec{k}$ because our contour planes are horizontal. For any general plane we would have to use some general normal vector $\vec{N}$. Neither the normal vectors origin nor magnitude are of consequence here so we have chosen a vector of length 1 starting at the true matrix origin.

Contouring Situation

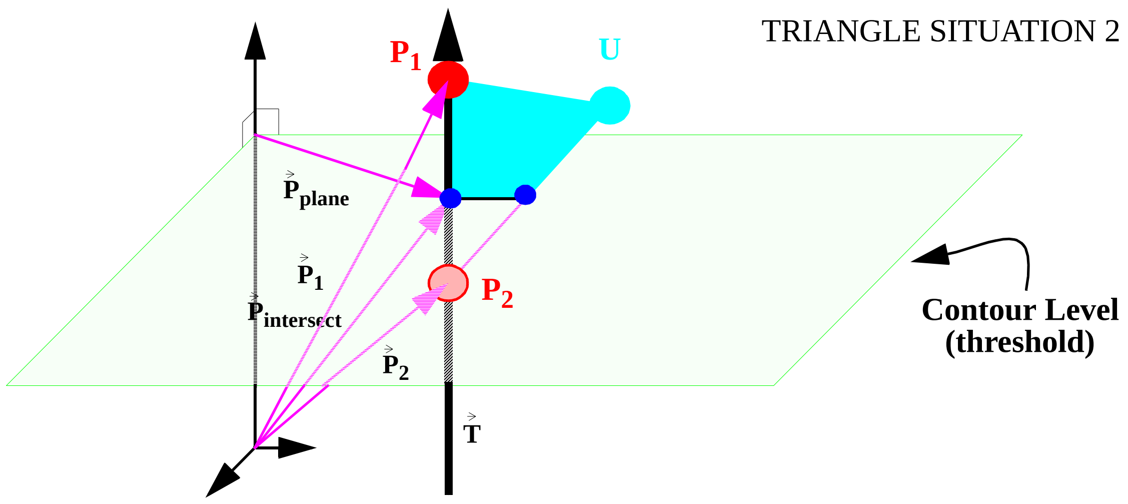


Figure 4-31 - Second type of intersection with a contour plane.

The line $\vec{T}$ is then described by

$$\vec{T} = c_1(\vec{P}_1 - \vec{P}_{intersect}) = c_2(\vec{P}_1 - \vec{P}_2) = c_3(\vec{P}_{intersect} - \vec{P}_2)$$

where c_i are any scalar values. For the intersection point, we have

$$\vec{P}_{intersect} = \vec{P}_1 + c'\vec{T}$$

We need now substitute $\vec{P}_{intersect}$ as described in the last equation into our equation for the contour plane.

$$\vec{P}_{plane} \bullet \vec{k} = 0$$

$$[\vec{P}_{intersect} - (threshold)\vec{k}] \bullet \vec{k} = 0$$

$$[(\vec{P}_1 + c'\vec{T}) - (threshold)\vec{k}] \bullet \vec{k} = 0$$

If we solve for the constant c'

$$[(\vec{P}_1 + c'\vec{T}) - (threshold)\vec{k}] \bullet \vec{k} = 0$$

$$[\vec{P}_1 \bullet \vec{k}] + [c'\vec{T} \bullet \vec{k}] - [(threshold)\vec{k} \bullet \vec{k}] = 0$$

$$c'\vec{T} \bullet \vec{k} = [(threshold)\vec{k} - \vec{P}_1] \bullet \vec{k}$$

$$c' = \frac{[(threshold)\vec{k} - \vec{P}_1] \bullet \vec{k}}{\vec{T} \bullet \vec{k}}$$

and then substitute this back into our equation for the intersection point we attain

$$\vec{P}_{intersect} = \vec{P}_1 + c'\vec{T} = \vec{P}_1 + \frac{[(threshold)\vec{k} - \vec{P}_1] \bullet \vec{k}}{\vec{T} \bullet \vec{k}}\vec{T}$$

Now we need only to described the line $\vec{T}$ in terms of quantities we already know to have a working formula for the intersection point. We choose the simplest description of $\vec{T}$

$$\vec{T} = c_2(\vec{P}_1 - \vec{P}_2) = (\vec{P}_1 - \vec{P}_2)$$

Our equation is then

$$\vec{P}_{intersect} = \vec{P}_1 + \frac{[(threshold)\vec{k} - \vec{P}_1] \bullet \vec{k}}{(\vec{P}_1 - \vec{P}_2) \bullet \vec{k}}(\vec{P}_1 - \vec{P}_2)$$

and since the z-components are the (matrix) points themselves we have

$$\vec{P}_{intersect} = \vec{P}_1 + \frac{[threshold - P_1]}{P_1 - P_2}(\vec{P}_1 - \vec{P}_2)$$

where $\vec{k}$ is a (unit) vector along the z - direction and perpendicular to the contour level plane, and where $\vec{P}_0$ is any point (other that the intersection point) in the contour level plane. The second intersection point may be found by replacing point $\vec{P}_2$ with point $\vec{U}$ (or $\vec{L}$) in the previous equation.

As the matrix is scanned over a specific contour level (by investigating all of the possible triangles), sets of two points are constantly passed to the function ***PL_contour***. These are stored in dual “matrices” of contour lines for the level being contoured, one set which is increasing to the “left” and the other which is increasing towards the “right”. As contributors to the contour lines for the contour level being treated are found they are treated in three distinct ways.

I Points are not connected to any previous lines found - start a new contour line.

I Points are a continuation of a previous contour line - add it to existing contour.

I Points connect two previous contour lines - concatenate two existing lines into one.

I Points connect a previous contour to form a closed contour - output contour line.

PolyLines are stored, one branching off from the first point to the left and another branching off from the first contour point to the right.

4 MATLAB I/O

4.1 Overview

The MATLAB I/O routines are provided to allow the transfer of matrices between GAMMA and the program MATLAB[1].

4.2 Available MATLAB Functions

4.3 MATLAB Discussion

4.4 MATLAB Figures & Tables

1. MATLAB is a product of The MathWorks, Inc., 21 Eliot Street, South Natick, MA 01760. Phone: (508) 653-1415, Telex: 910-240-5521, FAX: (508) 653-2997, E-mail: na.mathworks@na-net.stanford.edu. GAMMA was written and used in conjunction with PRO-MATLAB for Sun Workstations, the most recent date on the supplied manual being Feburary 3, 1989.

4.5 Routines

4.5.1 MATLAB

Usage:

```
#include <MATLAB.h>
void MATLAB (const char* filename, const char* dataname, matrix &mx, int rc=1);
void MATLAB (File &file, const char* dataname, matrix &mx, int rc=1);
matrix MATLAB (const char* filename, const char* dataname);
```

Description:

The function MATLAB is used to read or write MATLAB MAT files, that is, files in the standard MATLAB format. The MATLAB file name is “filename”, typically something with a .mat suffix such as name.mat.

1. **MATLAB (const char* filename, const char* dataname, matrix &mx, int rc=1)** - When MATLAB is invoked with this argument list it writes the data contained in the matrix “mx” to a newly constructed file “filename” in the MATLAB MAT format. The data is given the MATLAB internal variable name “dataname”. If rc is set to zero only the real part of the matrix is output. If rc is 1 (default), both the reals and the imaginaries are written. The file is closed upon the function return and will overwrite any file “filename” previously in existance when the function is called.
2. **MATLAB (File &file, const char* dataname, matrix &mx, int rc=1)** - When MATLAB is invoked with this argument list it writes the data contained in the matrix “mx” in the MATLAB MAT format to wherever the file pointer “file” is at. The data is given the MATLAB internal variable name “dataname”. If rc is set to zero only the real part of the matrix is output. If rc is 1 (default), both the reals and the imaginaries are written. The file where “file” is pointing is assumed to be open when the function is called and will remain open with the file pointer advanced to the end at the function return. The file should be closed externally.
3. **MATLAB (const char* filename, const char* dataname)** - When MATLAB is invoked with this argument list it attempts to read the file “filename”, assumed in the MATLAB MAT format, and retreive the data “dataname”. The name “dataname” is the variable name which MATLAB uses internally.

Note that MATLAB can be called with a 1 or 2 dimensional data block in place of the matrix (block_1D or block_2D). MATLAB mat files are typically named with a “.mat” suffix so it is recommened that all filenames used for this function end with .mat.

Return Value:

Nothing when producing a MATLAB file, a matrix when reading a MATLIB file.

Example:

```
#include <gamma.h>
main ()
 {
 File fp;                                   // Specify a file pointer
 fp.open(“twomxs.mat”,io_writeonly,a_create);// Open file twomxs.mat
 matrix mx(101,101);                        // Define a matrix
 block_1D BLK(101), BLK1(101);              // Define two 1D-data blocks
 BLK = sinc(101, 50, 10);                   // First block to sinc function
 for(int i=0; i<101; i++)                   // Fill matrix with sinc by sinc
  for(int j=0; j<101; j++)
   mx(i,j) = BLK(i) * BLK(j);
 MATLAB(“onemx.mat”, “mx1”, mx, 0);         // Output MATLAB file onemx.mat, reals
 MATLAB(fp, “mx1”, mx);                     // Put matrix into file twomxs.mat, complex
 BLK1 = square_wave(101, 20, 70);           // Fill block with box function
 for(int k=0; k<101; k++)                   // Fill matrix with sinc x box
  for(int l=0; l<101; l++)
   mx(k,l) = BLK(k) * BLK1(l);
 MATLAB(fp, “mx2”, mx);                     // Put matrix into file twomxs.mat
 fp.close();                                // Close file twomxs.mat
 matrix mx2;                                // Define a second matrix for fun
 mx2 = MATLAB(“twomxs.mat”, “mx2”);         // Read file twomxs.mat, retreive mx2
 }
```

In this example, a file onemx.mat is produced contaning a single matrix in the MATLAB MAT format. A second file, twomxs.mat, is also produced which contains two matrices useable by MATLAB. In this latter case the user opens and closes the file directly and is able to write multiple matrices into it. This is not true for the first file which is produced with a single line of code and may contain only one matrix. Finally, the second file is re-opened and scaned for the variable “mx2”, the second matrix. This is put into the matrix mx2 but unused in the example.

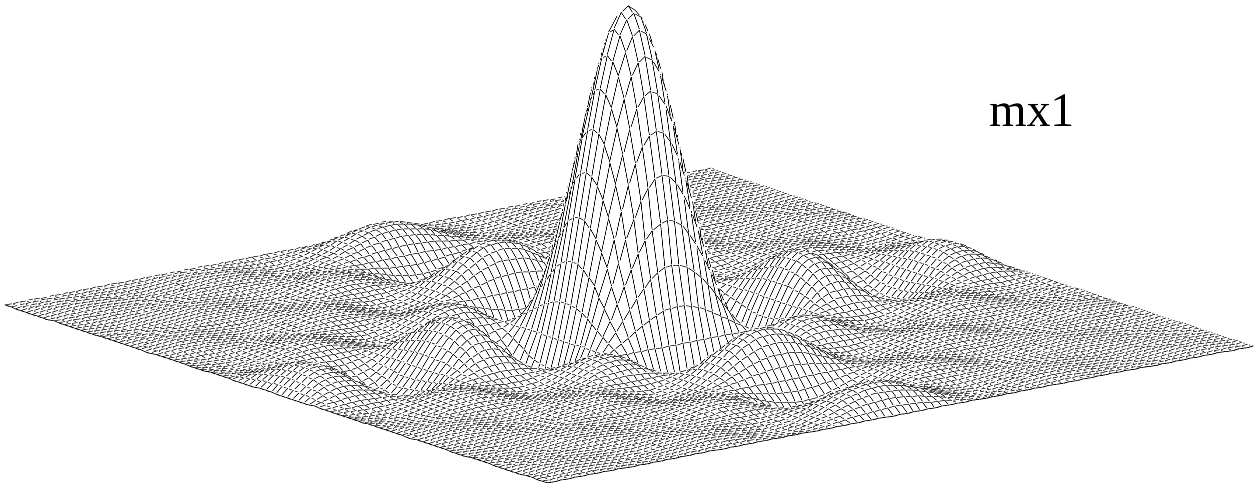
To see a mesh plot of the data contained in “twomxs.mat” issue the following commands within MATLAB-

- load twomxs - Load in the file. This may need the directory path as well, e.g. load /nmrnet/home/sosi/twomxs.
- mesh(mx1) - Graph the first matrix as a meshed 2D-plot.
- mesh(mx2) - Graph the second matrix as a meshed 2D-plot.

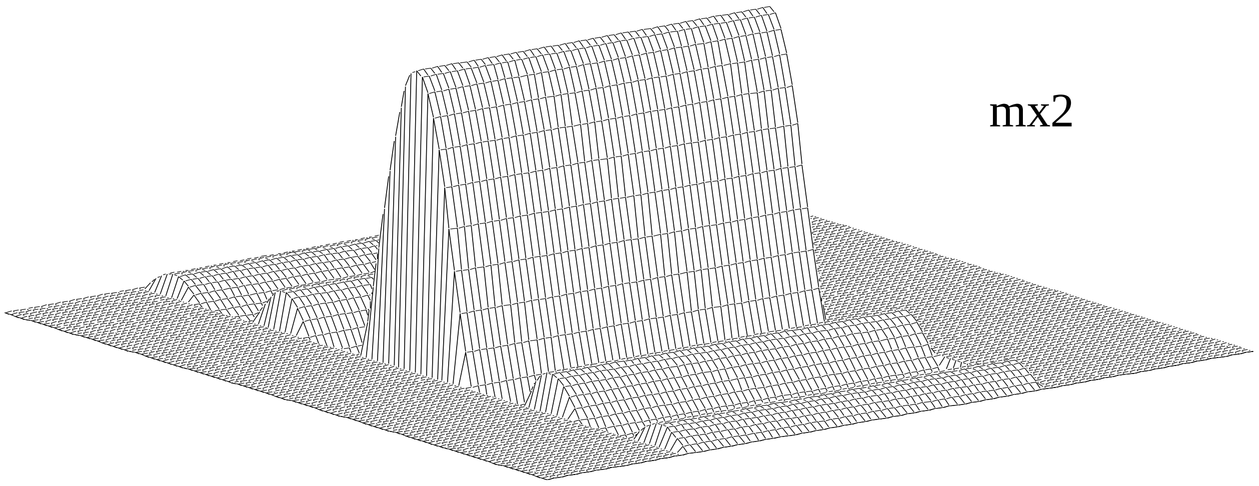
mesh(mx2) - Have MATLAB produce a mesh plot of the matrix mx2.

MATLAB plots may be incorporated into FrameMaker if desired. Currently, the MATLAB plot must be output as a MATLAB meta file, converted to HPGL format with the MATLAB supplied program gpp, then converted to encapsulated postscript with the FrameMaker supplied program hpgltoeps, and finally imported into the FrameMaker document of choice. Note that each MATLAB plot must be output to a separate meta file or the plots will overlap in FrameMaker. The following plots were produced in this manner from the file twomxs.mat created in the example. They have been resized and labeled after importing.

MATLAB Example Plot 1



MATLAB Example Plot 2



By default, the northwest corner is the matrix point (0,0) and the southwest corner (0,ncols-1). The MATLAB commands (here separated by semicolons for brevity)

```
load twomxs; mesh(mx1); meta MLmx1; mesh(mx2); meta MLmx2; exit;
```

produce the two MATLAB meta files MLmx1 and MLmx2. These are subsequently converted to hpgl format by the commands issued in UNIX (again separated by semicolons for brevity)

```
gpp MLmx1 -dhpgl; gpp MLmx2 -dhpgl
```

which takes the MAT files and produces HPGL plot files MLmx1.hpgl and MLmx2.hpgl. These are then converted to encapsulated postscript by issuing the commands from UNIX

```
hpgltoeps MLmx1.hpgl MLmx1; hpgltoeps MLmx2.hpgl MLmx2
```

which creates the two files MLmx1 and MLmx2. These are plotted above and were incorporated into this document using the Import option under File at the top of the document in FrameMaker.

4.6 Description

4.6.1 MATLAB “MAT” File Structure

MATLAB always maintains its data as matrices and each MATLAB MAT file may contain several matrices. Internally, each matrix is preceeded by a header which contains the information reguarding the data size, the matrix name, and so forth. This scheme is depicted in the figure below.

MATLAB MAT File Structure

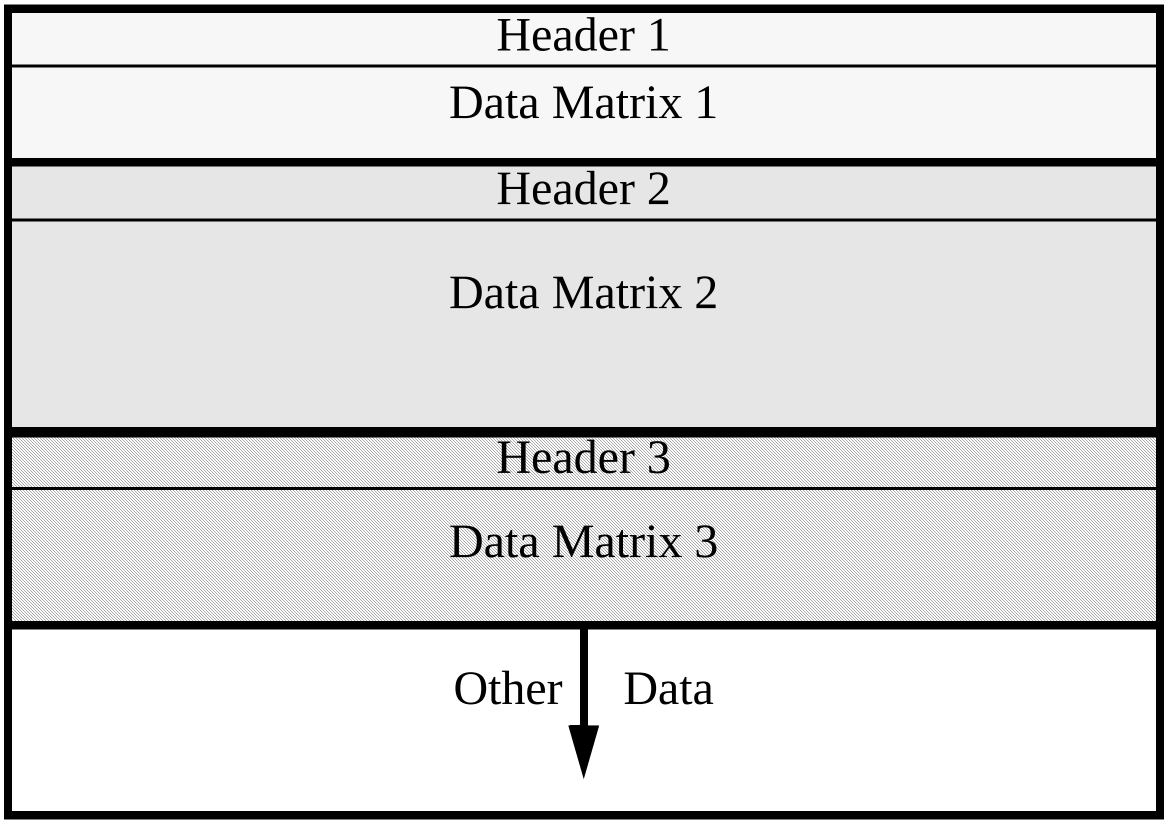


Figure 25-1 - Overall file structure of a MATLAB MAT file containing multiple matrices.

4.6.2 MATLAB “MAT” File Header Structure

The header structure is described in the MATLAB manual under load, save in the Reference Chapter, page 3-75 in the PRO-MATLAB August 1987 version. Essentially each header is a 20 byte structure containing 5 four-byte long-integers (words) as depicted below

MATLAB MAT Header Structure

type	mrows	ncols	imagf	namlen

Figure 25-2 - Header Structure of a MATLAB MAT file.

The five parameters are defined as follows.

type - Type flag. An integer indicating the computer type the data was produced on.

mrows - Row dimension. An integer with the number of rows in the stored matrix.

ncols - Column dimension. An integer with the number of columns in the matrix.

imagf - Imaginary Flag. Real data: imagf=0; Complex data: imagf=1.

namlen - Name Length. Integer = number of characters in variable name + 1.

4.6.3 MATLAB “MAT” File Data Structure

The structure of the stored matrix data is described in the same section of the MATLAB manual previously cited for the header structure. The size will of course vary depending upon how much data is stored but there is always the data name followed by the real data and then optionally followed by the imaginary data (if present).

MATLAB MAT Matrix Data Structure

variable name	real data	imaginary data (optional)

Figure 25-3 - Matrix data structure of a MATLAB MAT file.

The three sections are construcated as follows.

var. name- namlen ASCII bytes (characters). The last is a NUL (or 0).

reals - mrow*mcol double precision floating point numbers (8-bytes each).

imags - Stored identically as the real data. Immediately following the last real point.

MATLAB matrices are stored column-wise (unless indicated otherwise by type). This means that the first data point (immediatly after the variable name) will correspond to the matrix point (0,0). The second point is (1,0), the third (2,0) and so on.

For a general discussion on moving files in and out of MATLAB see Importing and exporting data in the Tutorial Chapter, Section 12 on page 2-83 in PRO-MATLAB August 1987 version.

5 Felix I/O

5.1 Overview

The Felix I/O routines are provided to allow the transfer of spectra between a Felix[1] file and GAMMA. A few routines for reading files from the predecessor of Felix, FTNMR, are also included here. Felix I/O routines will be preferentially enhanced and users should attempt to replace the use of FTNMR with Felix entirely. WARNING: Felix is a finicky program which is being constantly altered by its creators. The file structures read and produced by Felix, if altered, may render many (if not all) of these functions useless on later Felix versions.

5.2 Available Felix Functions

Reading and Writing Felix .dat Files

Felix	- Write a Felix .dat file	page 75
Felix_1D	- Read a Felix .dat file into a GAMMA vector	page 81
Felix_2D	- Read a Felix .dat file into a GAMMA matrix	page 82
Felix_header	- Read the header of a Felix.dat file	page 84
Felix_d_cat	- Read a concatenated Felix .dat file into a GAMMA matrix	page 85

Reading and Writing Felix .mat Files

Felix_mat	- Write a Felix .mat file	page 90
Felix_mat_1D	- Read a Felix .dat file into a GAMMA vector	page 90
Felix_mat_header	- Read a Felix .dat file into a GAMMA matrix	page 91

5.3 Discussion of Felix

1. Felix is an NMR data processing program from Hare Research, Inc., 14810 216th Avenue NE, Woodinville, WA., 98072, USA. Version 1.0 was used in preparation and testing of these subroutines. All examples were performed on a SUN SPARCstation under SUNViews. Any references to the Felix manual is for the March, 1990 copy.

5.4 Felix Figures & Tables

5.5 Routines

5.5.1 Felix

Usage:

```
#include <Felix.h>
void Felix (const char* filename, block_1D &BLK, int rc=1);
void Felix (const char* filename, block_2D &BLK, int rc=1);
void Felix (File &fp, block_1D &BLK, int rc=1, int reset=0);
```

Description:

The function ***Felix*** is used to write Felix ".dat" (or serial) files. The data to be written in is contained in either a one-dimensional or two-dimensional data block ***BLK***. The Felix output file is specified either by a file name ***filename*** or by a pointer to an open file ***fp***. The parameter ***rc*** specifies whether real or complex data is written. For real, ***rc*** = 0, and for complex ***rc***=1. This will default to complex if left out of the function argument list.

1. **Felix (const char* filename, block_1D &BLK, int rc=1)** - When ***Felix*** is invoked with this argument list it writes the data contained in the 1-dimensional data block ***BLK*** to a newly constructed file ***filename*** in the Felix .dat format. If ***rc*** is 1 (default) the data is written as complex numbers. If ***rc*** is set to zero, only the real data of the block is output. Any parameters in ***BLK*** compatible with the Felix parameters will be automatically transferred into the Felix file. The output file is closed upon the function return. The function will overwrite any file ***filename*** previously in existence.
2. **Felix (const char* filename, block_2D &BLK, int rc=1)** - This function is similar to the use above (with 1D data blocks) but writes the data contained in the 2-dimensional data block ***BLK***. This is done row-wise, i.e. first row 1 of ***BLK*** is written followed by row 2 and so on until the end of the data in ***BLK***.
3. **Felix (File &file, block_1D &BLK, int rc=1)** - When ***Felix*** is invoked with this argument list it writes the data contained in the 1-dimensional data block ***BLK*** in the Felix .dat format to wherever the file pointer ***file*** is at. The file where ***file*** is pointing is assumed to be open (opened explicitly sometime prior to the function call) and will remain open with the file pointer advanced to the file end at the function return. The file should be closed externally as well. The flag ***reset*** tells the program whether or not to write any header information. If you do not desire the header information to be written in the Felix .dat file then this is inconsequential. If your program has not called a Felix function in connection with another file then this is unimportant. If you want the header and have used function Felix earlier in your program to generate a file then you must "reset" the Felix function to tell it the header should be output. For this, ***reset*** is set to a non-zero number on the first, and only the first, function call (on the newly opened file attached to fp).

Felix dat files are typically named with a ".dat" suffix so it is recommend that all filenames used for this function end with .dat. Furthermore, Felix has trouble recognizing capitol letters (at least in UNIX) so filenames should be all lower case letters.

* Note: Felix has difficulties with real data. It is now mandatory that the user specifies the data set is real within Felix itself.

Return Value:

Nothing. A new disk file in Felix ".dat" format is produced.

Example 1:

For this first example the function is used to output a 1D NMR spectrum. The data block “data” is filled with the simulated FID of a two spin system following a simple 90 degree pulse.

```
#include <gamma.h>
main ()
 {
 spin_system ab(2);                              // Create a spin system with 2 spins
 ab.shift(0,-700.5);                             // Set chemical shift of fist spin to -700.5 Hz
 ab.shift(1,+600);                               // Second spin to 600 Hz
 ab.J(0,1,20);                                   // Coupling to 20 Hz
 gen_op sigma, H, detect;                        // Declare the operators
 sigma = sigma_eq(ab);                           // Set the density matrix to equilibrium
 H = Ho(ab);                                     // Set isotropic liquid Hamiltonian
 detect = Fm(ab);                                // Set the detection operator to F-
 lock_1D data(2048);                             // Declare a block for data
 sigma = Iypuls(ab,sigma,PI/2);                  // Apply a (PI/2) y pulse
 FID(sigma, detect, H, 0.0005,2048, data);       // Calculate the FID after the pulse
 Felix(“felix.dat”, data);                       // Output the Felix .dat file
 }
```

The last line of the program creates the file felix.dat readable by Felix. The file contains a complex FID which is worked up in Felix to produce an NMR spectrum. The commands and spectrum (from Felix) are shown below.

Felix 1D Spectrum Output

1. re felix.dat
2. lb 5
3. em
4. ft
5. ref 1024
6. ax 2
7. dr

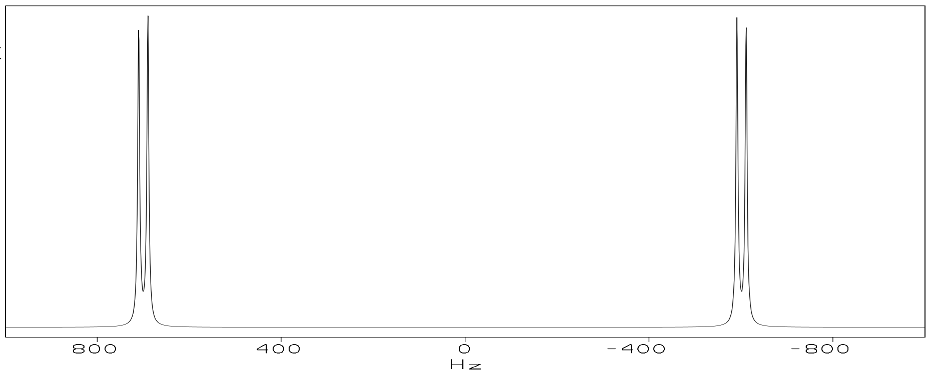


Figure 4-1 - Example program result from use of the GAMMA function “Felix”.

Example 2:

This example shows how the function is utilizes a 2D-data array (either a block_2D or a matrix) to produce a Felix .dat file. To keep the program simple, the data block BLK is filled with the product of a sinc and sinusoidal function.

```
#include <gamma.h>
main ()
 {
 block_2D BLK(256,256);                  // Declare a 2D data block
 block_1D BLK1(256);                     // Declare a 1D data block
 BLK1 = sinc(256, 128, 10);              // Set the 1D block to a sinc function
 for(int i=0; i<256; i++)                // Fill the 2D block with sinc(x)*sinc(y)
  for(int j=0; j<256; j++)
   BLK(i,j) = BLK1(i) * BLK1(j);
 Felix("felix.dat", BLK);                // Write Felix .dat file (a serial file)
 }
```

As in the previous example, the last line of the program creates the file felix.dat readable by Felix.

Felix 2D Spectrum Serial Output

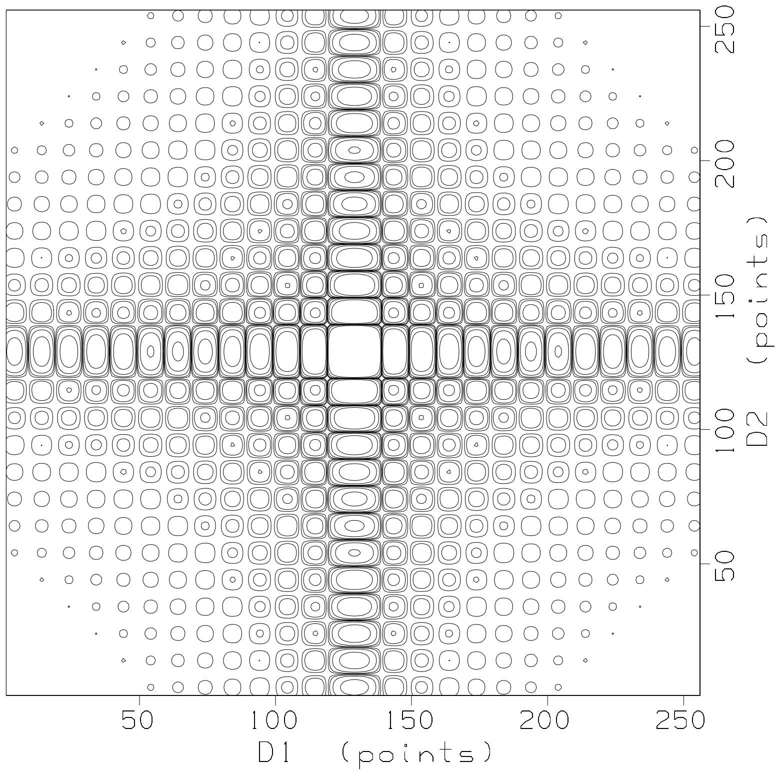


Figure 4-2 - Example program result from use of the GAMMA function “Felix”.

Each data row is successively written so that Felix can read them in the .dat format. For the above plot, felix.dat was read into a Felix matrix with a macro and then contoured. An hpgl output file was then produced from Felix and transformed into encapsulated postscript(eps) with a program provided by FrameMaker. The eps file was imported into this document (in FrameMaker) and resized. The Felix macro which produced the matrix file is as follows (the comments off to the side are not part of the macro) -

```
bld felix 2 256 256 1! build a felix 2D matrix, 256x256 real
mat felix.mat write! open the matrix created for writing
for row 1 256! loop through each row of the matrix
re felix.dat! successively read each row of the .dat file
red! set the row to be real, not complex
sto 0 &row! store the row in the matrix
typ row=&row! write to standard output this has been done
next! go back for the next row
end
```

Once this macro has been executed in Felix, the commands to produce the contour plot on the screen are[1] -

```
lvl 0.000000001! set contour level very low (10**8 lower than exptl.)
cpn 1! both positive and negative contours
nl 5! five levels
cli 1! geometrically progressing contours
clm 2.5! contours increment 250 percent
cp! draw the contour plot to the screen
```

To generate the hpgl contour plot file, the Felix commands are (once cp produces the screen plot)

```
hdv felix.hpgl! hardcopy device is file felix.hpgl
hpm 32! hardcopy plot mode is hpgl
hcp! produce the plot
```

Finally to produce the encapsulated postscript file for importing into FrameMaker, the program hpgltoeps provided by FrameMaker was used. This is done outside of Felix (in UNIX) and the command was

```
hpgltoeps felix.hpgl felix.eps
```

and produced the file felix.eps that was incorporated for the plot on the previous page.

1. Felix version 1.0 seems to prefer that one draws 1D plots before 2D plots or it confuses itself on the plot limits. Apparently loading a row (loa 0 256) and drawing it (dr) then loading a column (loa 130 0) and drawing it prior to the contour plot does something to help Felix figure itself out.

Example 3:

This example demos use of function Felix in a loop, writing successive 1-D blocks to a serial file.

```
#include <gamma.h>
main ()
 {
 block_1D BLK1(128), BLKA(128), BLKB(128);    // Create 3 1-D data blocks
 BLK1 = Gaussian(128, 32, 42.46);             // Set BLK1 to a Gaussian
 BLKA = sinc(128, 64, 12);                    // Set BLKA to a sinc
 File fp;                                     // Create a file
 fp.open("felix.dat", io_writeonly, a_create);  // Open file with name felix.dat
 for(int i=0; i<128; i++)                     // Loop over 128 points, filling
  {                                           // the block BLKB with a blend
  BLKB = i*BLKA + (127-i)*BLK1;               // of the Gaussian and sinc then
  Felix(fp, BLKB);                            // write the result block to the
  }                                           // file in Felix .dat format
 fp.close();                                  // Close the file[1]
 }
```

Felix 1D Spectrum Output

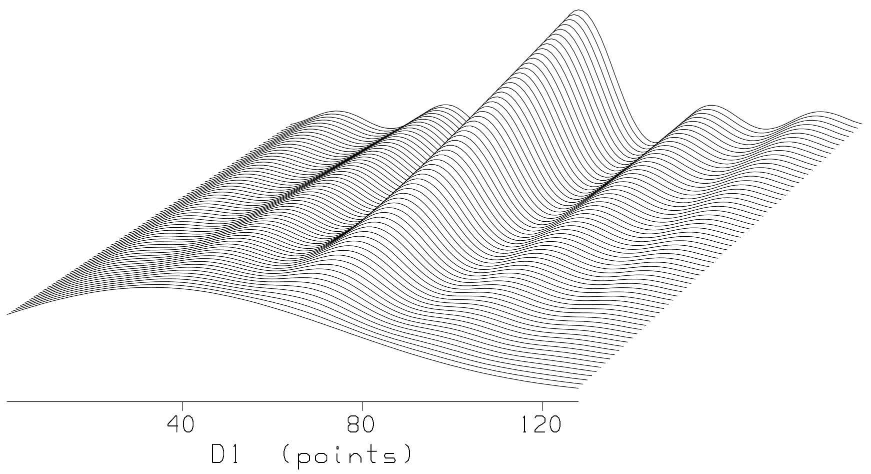


Figure 4-3 - Example program result from use of the GAMMA function "Felix" in a loop.

1. If this program were to continue and generate some other Felix .dat file using this same form of the function Felix, the "reset" flag would have to be used on the first function call if any parameters are to be written to the file. The same would be true in this program had any of the forms of function Felix been called previous to where it is called in the loop. To set the "reset" status, the loop would then go from 1 to <128 and the first row (0) output before the loop with Felix(fp,BLKB,1,1) where the last 1 tells the program to write the header information. If this is not done, the header will simply not be written and the program still works fine.

In this example the file felix.dat is produced from first opening the file then successively writing 128 1D data blocks to it. For the above plot, felix.dat was read into a Felix matrix with a macro and then appropriate parameters were set for a reasonable stack plot. An hpgl output file was then produced from Felix and transformed into encapsulated postscript(eps) with a program provided by FrameMaker. The eps file was imported into this document (in FrameMaker) and resized. The Felix macro which produced the matrix file is as follows (the comments off to the side are not part of the macro) -

```
bld felix 2 128 128 1! build a felix 2D matrix, 128x128 real
mat felix.mat write! open the matrix created for writing
for row 1 128! loop through each row of the matrix
re felix.dat! successively read each row of the .dat file
red! set the row to be real, not complex
sto 0 &row! store the row in the matrix
typ row=&row! write to standard output this has been done
next! go back for the next row
end
```

Once this macro has been executed in Felix, the commands to produce the contour plot on the screen are[1] -

```
loa 0 128! load the last row of data
dr! have a look at the row on the screen
loa 50 0! load the 50th column of data
dr! have a look at the column on the screen
dx 0.4! set the x-axis skew
dy 0.4! set the y-axis skew
sp! generate the stack plot on the screen
```

To generate the hpgl contour plot file, the Felix commands are (once cp produces the screen plot)

```
hdv felix.hpgl! hardcopy device is file felix.hpgl
hpm 32! hardcopy plot mode is hpgl
hcp! produce the plot
```

Finally to produce the encapsulated postscript file for importing into FrameMaker, the program hpgltoeps provided by FrameMaker was used. This is done outside of Felix (in UNIX) and the command was

```
hpgltoeps felix.hpgl felix.eps
```

and produced the file felix.eps that was incorporated for the plot on the previous page.

1. Felix version 1.0 seems to prefer that one draws 1D plots before 2D plots or it confuses itself on the plot limits. Apparently loading a row (loa 0 128) and drawing it (dr) then loading a column (loa 50 0) and drawing it (dr) prior to the stack plot does something to help Felix figure itself out. The manual claims at least one should be done to set the scaling, but if not done half of the data matrix disappears

5.5.2 Felix_1D

Usage:

```
#include <Felix.h>
block_1D Felix_1D(const char* filename, int block=0);
```

Description:

The function ***Felix_1D*** is used to read a 1-dimensional spectrum from a Felix ".dat" file. The Felix file name is ***filename***, typically something with a .dat suffix such as name.dat. The spectrum (assuming there are more than one present in the file) is specified by the value of ***block*** which defaults to 0, the first spectrum. Note that, for N total spectra, the spectra are indexed from [0, N-1].

Return Value:

Nothing. A block_1D is returned containing the spectrum ***block*** from the Felix dat file ***filename***.

Example:

```
#include <gamma.h>
main ()
 {
 block_1D BLK = Felix("felix.dat");           // Get the first spectrum from felix.dat
 FM_1D("felix1.mif", BLK);                    // Output spectrum to FrameMaker
 BLK = Felix("felix.dat", 127);               // Get the 128th spectrum in felix.dat
 FM_1D("felix2.mif", BLK);                    // Output spectrum to FrameMaker
 }
```

Felix 1D Example Output

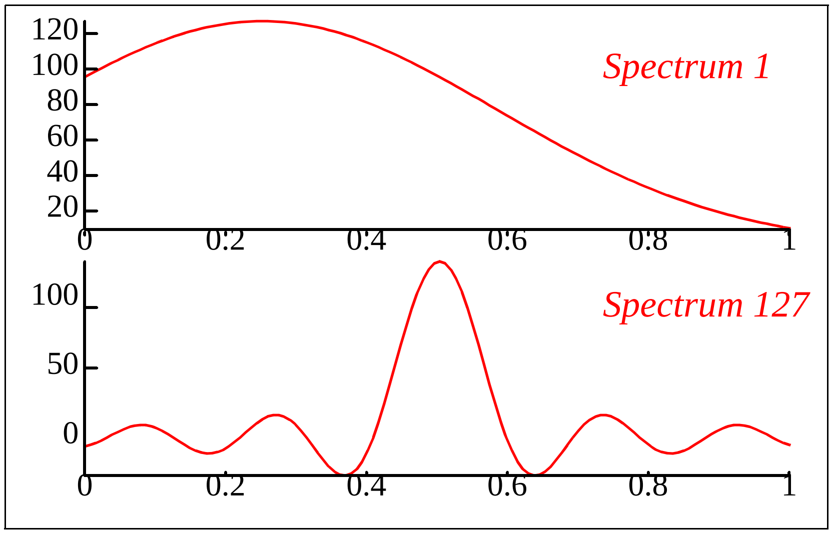


Figure 4-4 - Example program result from use of the GAMMA function "Felix" to read a file.

The example reads two 1_D spectra from a Felix .dat file. This was applied to the file which was generated and plotted in Example 3 for the function Felix on an earlier page of this document.

5.5.3 Felix_2D

Usage:

```
#include <Felix.h>
block_2D Felix_2D (const char* filename, int rowi =0, rows =0);
```

Description:

The function ***Felix_2D*** is used to read a 2-dimensional spectrum from a Felix ".dat" file. The Felix file name is ***filename***, typically something with a .dat suffix such as name.dat. The 2D spectrum can be only part of a larger data set, either 2D or ND. To read a sub-matrix, the initial and number of rows to be read can be specified with the parameters ***rowi*** and ***rows*** respectively. These both have default settings of zero to indicate that the entire .dat file should be read as a single 2D matrix. If only rows is left 0, it is assumed that the 2D matrix should be filled with the data from ***rowi*** until the end of the file. Both ***rowi*** & ***rows*** must be positive.

Return Value:

Nothing. A block_2D is returned containing a data array from the Felix .dat file "filename".

Example:

```
#include <gamma.h>
main ()
 {
  block_2D BLK;                              // Create a 2-D data block
 BLK = Felix_2D("felix.dat", 29, 79);        // Get the first spectrum from felix.dat
 FM_stack("felix.mif", BLK. 0.3, 0.3);       // Output spectrum to FrameMaker
 }
```

Felix 2D Example Output

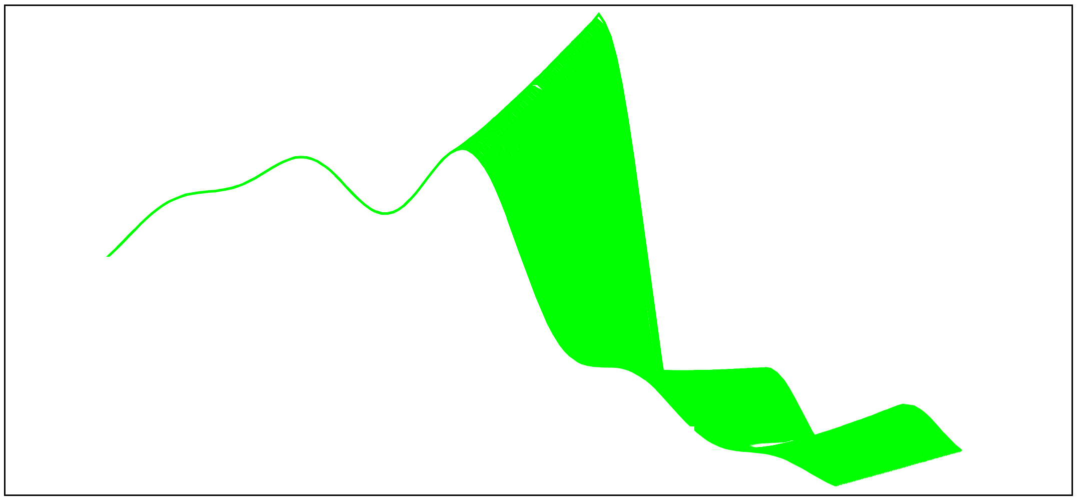


Figure 4-5 - Example program result from use of the GAMMA function "Felix_2D".

In this example, spectra 30 through 80 in the Felix.dat file felix.dat are read into a 2D-data block. A stack plot for FrameMaker is then output and shown above. The file was that used in Example 3 for the function Felix on an earlier page of this document.

5.5.4 Felix_header

Usage:

```
#include <Felix.h>
void Felix_header (const char* filename);
```

Description:

The function ***Felix_header*** is used for viewing the header information in a Felix file. Unlike its predecessor, FTNMR, the current version of Felix uses very little of the header information present. Felix does read the header and perhaps more of the information present will be used in future versions.

Return Value:

Nothing. Felix header information is written to standard output.

Example:

```
#include <Felix.h>
#include <String.h>// Could just have used #include <gamma.h>
 main ()
  {
  String filename;                          // Declare a string for the filename
  cout << “\n\tWhich Felix .dat File? “;    // Ask the user to give the filename
  cin >> filename;                          // Input the filename from the user
  cout << “\n”;                             // Output a linefeed so screen stays nice.
  Felix_header(filename);                   // Output the header information in the file
  cout << “\n”;                             // Output a linefeed so screen stays nice.
  }
```

Below is a sample of the output to expect from this function from a typical Felix.dat file.

```
Which Felix .dat File ? felix.dat
Initial integer read for FORTRAN = 32772
Header Size in Complex Points = -4096

  1. 4096                     Number of Complex Points
  2. 1                        Data Type = Complex
  3. 0                        Transform State = FID
  4. 0                        W2 Axis Type = None
  5. 0                        W2-W1 Axis Equivalence
  6. 0                        W1 Axis Type = None
  7. 0                        Empty
  8. 0                        Empty
  9. 0                        Empty
 10. 0                        Empty
```

11. 0	Pointer to Comments
12. 0	Length of Comments
13. 0	Pointer to Raw Header
14. 0	Length of Raw Header
15. 0	Spectrometer Type
16. 0 Hz.	W2 Spectral Width
17. 0 Hz.	W2 Spectrometer Frequency
18. 0	W2 Reference Point
19. 4096 MHz.	W2 Reference Frequency
20. 0	W2 Reference Frequency Type
21. 0 Deg.	W2 Zero Order Phase Correction
22. 0 Deg.	W2 First Order Phase Correction
23. 0	W2 First Order Phase Correction
24. 0 Hz.	W1 Spectral Width
25. 0 MHz.	W1 Spectrometer Frequency
26. 0	W1 Reference Point
27. 0 Hz.	W1 Reference Frequency
28. 0	W1 Reference Frequency Type
29. 0 Deg.	W1 Zero Order Phase Correction
30. 0 Deg.	W1 First Order Phase Correction
31. 0	Reserved
32. 0	Reserved

Final integer read for FORTRAN = 32772

5.5.5 Felix_d_cat

Usage:

```
#include <Felix.h>
block_2D Felix_d_cat(const char* filename, int IOout=0);
```

Description:

The function ***Felix_d_cat*** is used for reading a concatonated Felix .dat file, ***filename***. This function is similar to the function ***Felix_2D*** but it ignores any (or multiple) headers found in the file. This allows users to blend multiple .dat files into one by using standard UNIX file concatonation: ***cat file1.dat file2.dat > filename***. Once the concatonated data is an a GAMMA matrix it can be easily manipulated. The argument ***IOout***, if set to non-zero, will write information to standard output about the concatenated file as it is being processed

One example of this functions utility would be if a computer simulation does not run to completion. The job can be restarted in the middle and the two output Felix .dat file concatonated. This function can then effectively reproduce the full file.

This function is also handy when one has multiple Felix .dat files which the user desires to manipulate these together. The Felix write command (wr) is one means to get Felix to output specific .dat files which can then be blended together with this function.

Return Value:

Nothing. Felix header information is written to standard output.

Example:

The following program reads in a concatenated Felix.dat file, allows the user to manipulate it, the outputs the result into a FrameMaker stack plot. Note that the function is used early in the program, the rest of the code simply manipulates the data and spits out a FrameMaker plot.

```
# include <gamma.h>
main (int argc, char* argv[])
 {
 cout << "\n\tConcatonated Felix (.dat) File -> FrameMaker (.mif) Stack Plot\n";
 //                              Read in Filename & Felix File
 String filename;                                    // Name of spin system file
 query_parameter(argc, argv, 1,                      // Get filename from command
  "\n\tFelix concatonated .dat filename? ",  filename);// line or ask for it
 block_2D BLK = Felix_d_cat(filename, 1);            // Read Concatonated Felix .dat File
 //                  Alter the Concatonated Matrix Dimensions If Desired
 int nc = BLK.cols();
 int nr = BLK.rows();
 char yn;
 cout << "\n\tThe Concatonated Data Matrix is " << BLK.rows() << " By " << BLK.cols();
 cout << "\n\n\tDo You Wish to Plot Only Some of the Columns [y/n]? ";
 cin >> yn;
 int ic=0, ncols=nc;
 if(yn == 'y')
  {
  cout << "\n\tPlease Enter First Column Index [0, " << nc-2 << "]: ";
  cin >> ic;
  cout << "\n\tPlease the Number of Colums [2, " << nc-ic << "]: ";
  cin >> ncols;
  }
 cout << "\n\tDo You Wish to Plot Only Some of the Rows [y/n]? ";
 cin >> yn;
 int ir=0, nrows=nr;
 if(yn == 'y')
  {
  cout << "\n\tPlease Enter First Row Index [0, " << nr-2 << "]: ";
  cin >> ir;
  cout << “\n\tPlease Enter Last Row Index [2, “ << nr-ir << “]: “;
  cin >> nrows;
  }
 block_2D subBLK;
 subBLK = BLK.get_block(ir,ic,nrows,ncols);
 cout << “\n\tDo You Wish to Row Order Reversed [y/n]? “;
 cin >> yn;
 block_1D rowBLK1, rowBLK2;
 int kswap;
 if(yn == ‘y’)
  for(int k=0; k<nrows; k++)
   {
   kswap = nrows-k-1;
   if(kswap > k)
       {
       rowBLK1 = subBLK.get_block(k,0,1,ncols);
       rowBLK2 = subBLK.get_block(kswap,0,1,ncols);
       subBLK.put_block(kswap,0,rowBLK1);
       subBLK.put_block(k,0,rowBLK2);
       }
   }
 //                      Output FrameMaker .mif Stack File
 double xsize, ysize,  xsinc, ysinc;
 int rinc;
 cout << “\n\tPlease Enter Stack Plot Width in cm (8.5in = 21.5cm): “;
 cin >> xsize;
 cout << “\n\tPlease Enter Stack Plot Height in cm (11in = 27.9cm): “;
 cin >> ysize;
 cout << “\n\tPlease Enter Stack Plot Row Increment [1, nrows-1]: “;
 cin >> rinc;
 cout << “\n\tPlease Enter X Increment in cm: “;
 cin >> xsinc;
 cout << “\n\tPlease Enter Y Increment in cm: “;
 cin >> ysinc;
 FM_stack(“stack.mif”, subBLK, xsinc, ysinc, rinc, xsize, ysize);
 }
```

Concatonation of any two UNIX files is performed using the ***cat*** command as indicated in the function description. Subsequently, the concatonated Felix file can be read by a simple or, as in our example program, an elaborate GAMMA program. Worth mentioning is how to get Felix itself to produce a concatonated Felix .dat file from one of its matrix (.mat) files. This can by done with the following tricky but manageable macro (the comments off to the side are not part of the macro) -

```
get ‘First Matrix Row: ‘ rowi! get initial matrix row desired
get ‘Last Matrix Row: ‘ rowf! get final matrix row desired
for row &rowi &rowf! loop through matrix rows specified
loa 0 &row! load row into workspace
wr felblock.dat! write row to Felix .dat file named felblock.dat
sys felixcp! call to UNIX and concatonate with previous file
ty row = &row! echo that row is complete
next! go back for next row
end! exit the macro
```

After getting the matrix rows that the user wished concatonated, the macro loops through and writes each block to the file “felblock.dat”. Unfortunately, Felix does not append each successive block to what felblock.dat previously contained. It overwrites any data present so that at the end of each loop the output .dat file contains only one block (plus its header). Thus the macro also contains a call to the system to execute the command felixcp. Actually felixcp contains a couple of commands which concatenate felblock.dat to anything output previously. The file felixcp contains the following two lines (true UNIX commands):

```
cat subtot.dat felblock.dat > total.dat
cp total.dat subtot.dat
```

This first command concatenates the output Felix .dat file to the file subtot.dat and calls the result total.dat. The second line copies total.dat back over subtot.dat. At the beginning of the macro both subtot and total should be empty files and at end of the macro they will both contain all of the felblock.dat files concatenated together!

There are a few more things to know about this procedure. 1.) The files subtot.dat and total.dat must exist and be empty at the start of the macro. The four commands will accomplish this:

```
rm subtot.dat
rm total.dat
touch subtot.dat
touch total.dat
```

2.) The file felixcp should have executable privledges. This is done with the chmod command.

```
chmod u+x felixcp
```

3.) The file felixcp must reside in the default Felix directory. This will be the directory from which Felix is executed from.

4.) The two data files (subtot and total) must be in the Felix data directory. This is set with the following felix command (don’t forget to end with a slash):

```
pre dat /dir/subdir/
```

Thats all there is to it. You work up you data in a Felix matrix to get it into a desired format then execute the macro to spit out any need rows into a concatonated file. The following stack plot was produced in this fashion: 1.) GAMMA was used to perform a simulation (a decopuling experiment) which output an unprocessed Felix .dat file. 2.) Felix was used to process the simulated data into a Felix .mat file. 3.) The Felix macro listed previously was used to output the Felix matrix file into a concatenated Felix .dat file. The GAMMA program listed previously was used to read in the concatonated file and output a FrameMaker stack file, shown below.

Felix Concatonation Example Output

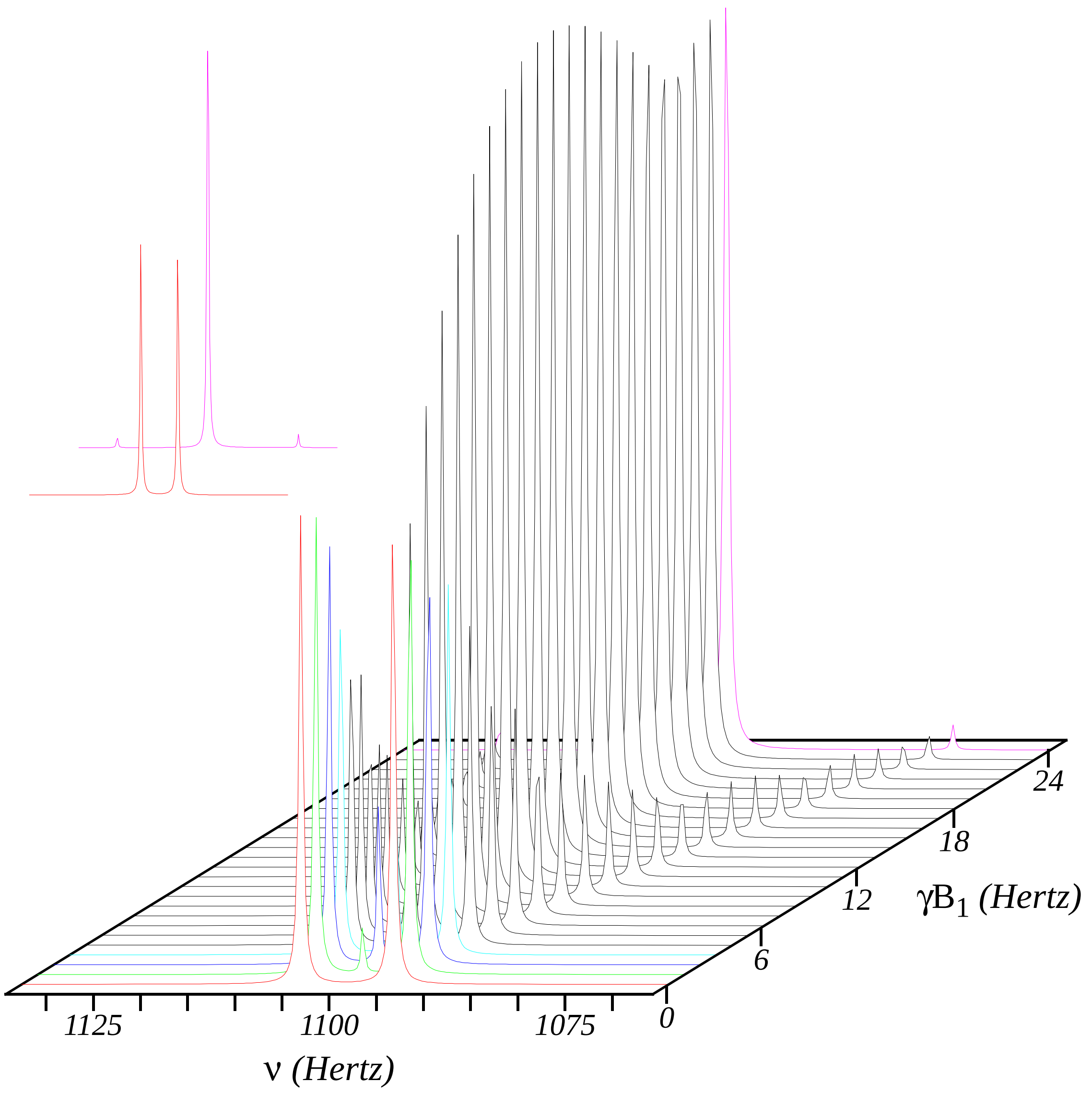


Figure 4-6 - Example program result from use of the GAMMA function “Felix_2D”.

It is preferable to use the Felix matrix functions provided, but if they fail this function can be very handy and perform the same feats with a bit of work.

5.5.6 Felix_mat

Usage:

```
#include <Felix.h>
void Felix_mat(const char* filename, block_2D &BLK, int rc=1);
void Felix_mat(File &fp, block_1D &BLK, int rc=1, int reset=0);
```

Description:

The function ***Felix_mat*** is used to write Felix ".mat" (or matrix) files. The data is contained in the data block ***BLK***. The file is specified either by a file name ***filename*** or by a pointer to an open file ***fp***. The parameter ***rc*** specifies whether real or complex data is written. For real, ***rc*** = 0, and for complex ***rc***=1. This will default to complex if left out of the function argument list.

1. **Felix_mat (const char* filename, block_2D &BLK, int rc=1)** - When Felix is invoked with this argument list it writes the data contained in the 2-dimensional data block ***BLK*** to a newly constructed file ***filename*** in the Felix .mat format. If ***rc*** is 1 (default) the data is written as complex numbers. If ***rc*** is set to zero, only the real data of the block is output. Any parameters in ***BLK*** compatible with the Felix parameters will be automatically transferred into the Felix file. The file is closed upon the function return. The function will overwrite any file ***filename*** previously in existence.
2. **Felix (File &fp, block_1D &BLK, int rc=1)** - When Felix is invoked with this argument list it writes the data contained in the 1-dimensional data block ***BLK*** in the Felix .mat format to wherever the file pointer ***fp*** is at. The file where ***fp*** is pointing is assumed to be open (opened explicitly sometime prior to the function call) and will remain open with the file pointer advanced to the file end at the function return. The file should be closed externally as well. The flag ***reset*** tells the program whether or not to write any header information. It is mandatory that the header information be present in the Felix .mat file (unlike a Felix .dat file where the header can be absent). This will be done automatically if your program has not previously called a Felix_mat function in connection with another file. If it has, then you must ***reset*** this Felix_mat function to tell it the header should be output. For this, ***reset*** is set to a non-zero number on the first, and only the first, function call to Felix_mat(on the newly opened file attached to ***fp***).

Felix mat files are typically named with a ".mat" suffix so it is recommend that all filenames used for this function end with .mat. Furthermore, Felix has trouble recognizing capitol letters (at least in UNIX) so filenames should be all lower case letters.

Return Value:

Nothing. A new file is produced in Felix .mat format.

Example:

5.5.7 Felix_mat_1D

Usage:

```
#include <Felix.h>
block_1D Felix_mat_1D (const char* filename, int block=0);
```

Description:

The function Felix_mat_1D is used to read a 1-dimensional spectrum from a Felix ".dat" file. The Felix file name is "filename", typically something with a .dat suffix such as name.dat. The spectrum (assuming there are more than one present in the file) is specified by the value of “block” which defaults to 0, the first spectrum. Note that, for N total spectra, the spectra are indexed from [0, N-1].

Return Value:

Nothing. A block_1D is returned containing the spectrum “block” from the Felix dat file “filename”.

5.5.8 Felix_mat_header

Usage:

```
#include <Felix.h>
void Felix_mat_header(const char* filename, int verbose=0);
```

Description:

The function ***Felix_mat_header*** is used for viewing the header information information in a Felix .mat file. The file name is input by ***filename*** and the amount of information to send out increases with the magnitude of the integer ***verbose***. There are 4096 integer length bits of information present in the header so the output can be quite long if verbose is set to maximim(>=10).

Return Value:

Nothing. Felix header information is written to standard output.

Example:

```
#include <gamma.h>
main ()
 {
 String filename;                          // Declare a string for the filename
 cout << “Which Felix .mat File ? “;       // Ask the user to give the filename
  cin >> filename;                         // Input the filename from the user
 cout << “\n\n”;                           // Output two linefeeds so screen stays nice.
 Felix_mat_header(filename);               // Output the header information in the file
 }
```

5.6 Description

5.6.1 Felix ".dat" File Structure

Each Felix .dat file is a serial type of file, i.e. a series of 1D spectra stacked one after another **which we will refer to as blocks**. At the beginning of each block are two integers. The first is used for structured I/O in FORTRAN (which Felix uses). The second is a flag as to whether or not the data in the block is spectral data (positive integer) or parameter data (negative integer). The absolute value of this second integer will be the number of complex points in the block, SIZE. There is no particular limit as to how many blocks are contained in a Felix .dat file (probably all data blocks should be of the same length). Each block also ends with an integer, again the result of FORTRAN sutructured I/O.

Felix .dat File Structure

A	+/-SIZE	0	1	· · · · · ·	SIZE-2	SIZE-1	A
A	-SIZE	0	1	· · · · · ·	SIZE-2	SIZE-1	A
A	SIZE	0	1	· · · · · ·	SIZE-2	SIZE-1	A
A	SIZE	0	1	· · · · · ·	SIZE-2	SIZE-1	A
				⋮ ⋮ ⋮ ⋮ ⋮ ⋮			

Figure 4-7 - File Structure of an Felix .dat file. There are SIZE complex points per each 1D spectrum. The integer A, which starts and ends each row, is used for FORTRAN structured I/O within Felix. The second integer of each row, +/- SIZE, if negative indicates that the row contains parameter information. The first data point of the row is indexed 0 and the last indexed size-1.

Felix ".dat" Header Structure - The first block in a Felix .dat file may contain parameters, not spectral data. This is indicated by the second integer in the block having a negative value. A header block can be of any size but normally (a Felix default) it will contain 32 complex values (64 floats or 64 integers). This default structure is shown in the following diagram.

Felix .dat File Header Structure

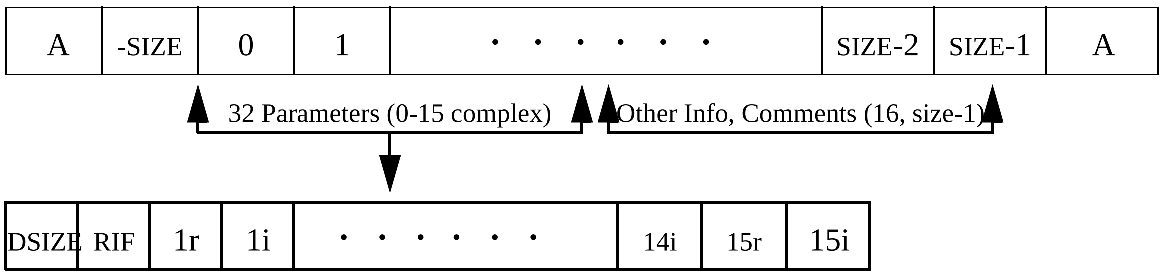

A
-SIZE
0
1
SIZE-2
SIZE-1
A
32 Parameters (0-15 complex)
Other Info, Comments (16, size-1)
DSIZE
RIF
1r
1i
14i
15r
15i

Figure 4-8 - Header Structure of an Felix .dat file. The first 16 complex points are used to store 32 parameters, either integer or real. The locations after this may be used for any additional parameters or comments. Although the program reads this information, Felix should be trusted only to use the 1st and 2nd parameters, the value of DSIZE and whether the data is real (RIF=0) or complex(RIF=1). Note that DSIZE in the header sets the number of points (real or complex) that Felix expects to read in ensuing data blocks, regardless of how much storage (SIZE) the block actually uses.

In principle, Felix uses the information contained in the header to set spectral parameters. In practice, some versions of Felix seem to have trouble maintaing this information (in the way that FT-NMR utilized it).

5.6.2 Felix ".dat" Data Structure

For all data blocks in a Felix .dat file the value stored in SIZE will always indicate the number of complex points stored in the block. A data block may contain either real or complex points, but this information is contained in the previous header block - the first non-data block in the .dat file. Also contained in the previous header block is the value DSIZE, the actual number of data points that Felix expects to obtain from the data block. Again, this information is independent from the value of SIZE. The number of data points used from a given block may actually be far less that the number of points stored in the block[1]. If the header has flagged the data as complex, the information is (expected to be) stored point-wise, that is re, im, re, im, ..., until the end. If the data contained in the block is real the points are stored in order, that is re, re, re, ..., until the end. The value DSIZE set by the previous header tells Felix how many points to take out of the data block. This value is the number of complex points to take when the data is complex and the number of real points to take when the data is real (unlike SIZE which is always assuming storage for complex points)[2]. Note: If no header exists (optional in Felix .dat files) the data is taken as complex and DSIZE=SIZE.

Felix .dat File Header Structure

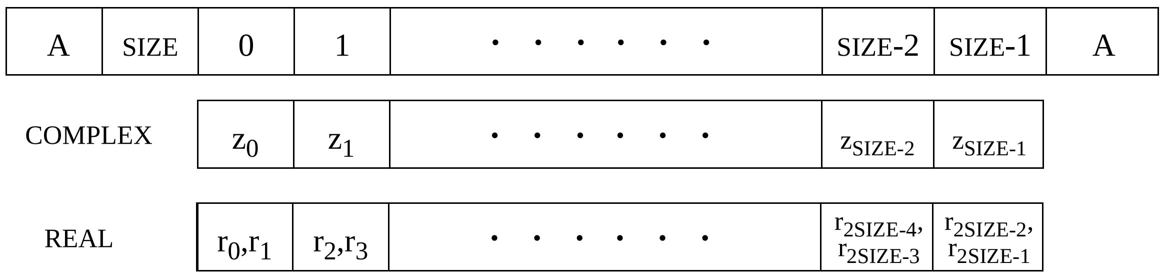


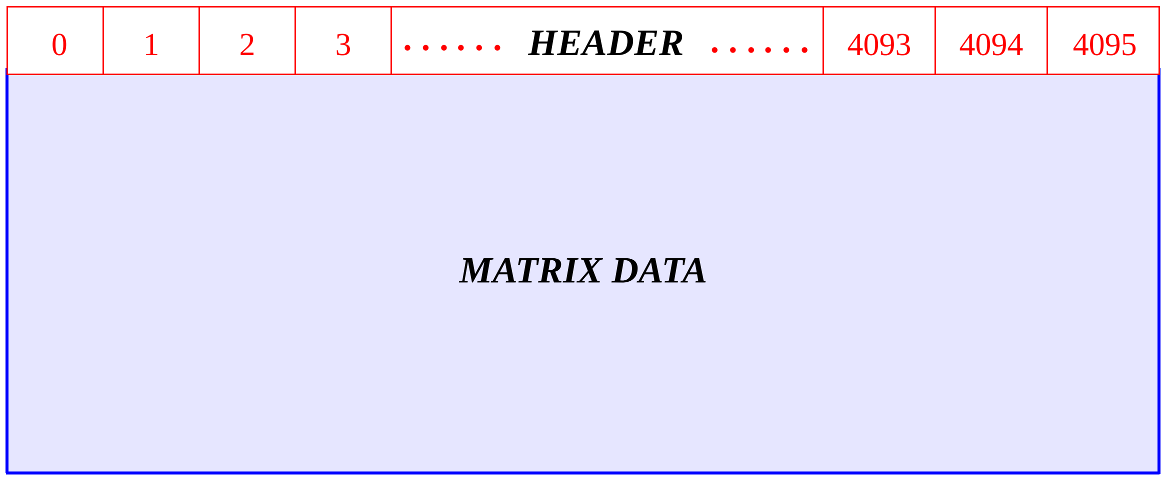
Figure 4-9 - Data Structure of an Felix .dat file. There are SIZE complex points or 2*SIZE individual real points. Complex points are stored real then imaginary. The storage of all reals versus complex is specified by the second parameter in the header. Felix may not use all of these points, that depends upon what the value of DSIZE was set to in the previous header block.

5.6.3 Felix ".mat" File Structure

Each file .mat internally consists of a header followed by the spectral data. Unlike a .dat file, there must be one (and only one) matrix header in each .mat file residing at the start of the file. It contains all parameters associated with the data set and is a block of integers, floats, and characters of length 4096. The matrix data points follow immediately after the header.

1. Why this is allowed is a mystery, as it wastes disk space. Fortunately, the number of points expected will not exceed the number which are stored!
2. This deviates from the program FTNMR. FTNMR always needs the number of complex points.

Felix .mat File Structure



5.6.4 Felix ".mat" File Header

As shown in the previous figure, the start of a Felix .mat file contains 4096 storage locations for parameters. These points are subdivided into four parts as shown in the following figure.

Felix .mat File Header Structure

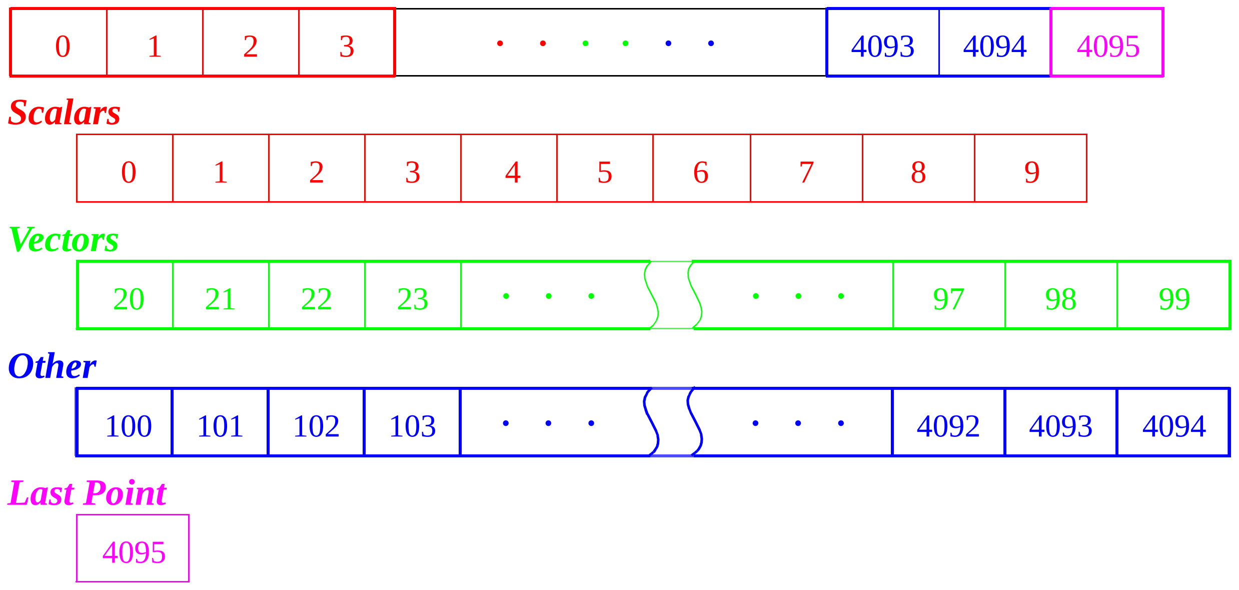


Figure 4-10 - Header Structure of an Felix .mat file. Note that the index in FORTRAN (the language in which Felix is written) is shifted by +1 realative to the standard C indexing used in GAMMA, that is vectors start at 21 and end at 100, etc.

Scalars - The initial header parameters are "scalar" parameters in that they are global matrix values, not assignable to any specific matrix dimension. For example, the flag indicating whether the data points are complex or real resides here. The following table describes these parameters.

Table 2: Felix .mat File Header Scalar Parameters

Point	Description of Scalar Paramters	Values	Variable
0	Matrix Dimensions	Min = 2, Max = 8	nd
1	Matrix Data Type	1 = Real, 2 = Complex	cmplx
2	Total Number Bricks in the Matrix[a]	Includes 1 for Header	brks
3	Bricks to Span Matrix Row Block[b]		blks
4	Unknown	Usually 0	
. .	. .	. .	. .

Table 2: Felix .mat File Header Scalar Parameters

Point	Description of Scalar Paramters	Values	Variable
19	Unknown	Usually 0	

a. A Felix .mat “Brick” is defined to be 4096 (4K) floating points.
b. A Felix .mat “Block” contains 64 floating points. This value is the number of Bricks which contains 64 matrix rows.

In most Felix .mat files (that the author has looked at) only the first four scalar values are present in the header. Below is a brief table of the first for scalar parameters found versus the matrix generated from the Felix bld command.

Table 3: Felix Matrices *versus* Felix Header Scalars

Felix bld Command	Scalar 0 Dimensions	Scalar 1 Type	Scalar 2 Bricks	Scalar 3 Blocks	Matrix Filesize	Matrix Points
bld test 2 512 512 0	2	1	65	8	1064960	262144
bld test 2 512 512 1	2	2	129	16	2113536	524288
bld test 2 256 512 0	2	1	33	8	540672	131072
bld test 2 512 256 0	2	1	33	8	540672	131072
bld test 2 256 512 1	2	2	65	8	1064960	524288
bld test 2 512 256 1	2	2	65	8	1064960	524288
bld test 2 32 1024 0	2	1	9	4	147456	32768
bld test 2 1024 32 0	2	1	9	4	147456	32768
bld test 2 32 1024 1	2	2	17	4	278528	65536
bld test 2 1024 32 1	2	2	17	4	278528	65536
bld test 2 32 32	2	1	2	1	32768	1024
bld test 3 32 32 8 0	3	1	5	2	81920	8192
bld test 3 32 8 32 0	3	1	5	2	81920	8192
bld test 3 8 32 32 1	3	2	5	2	81920	16384

As seen from the above table, the number of stored dimensions and the matrix data type is straightforward. A Felix brick is defined to be 4K real points, so the number of bricks can be determined by dividing the total matrix points by 4096 and adding in the header brick. The number of bricks which Felix uses can thus usually be determined by the formula

$$bricks = [(rpts/4096) + 1]$$

where $rpts$ is the total number of real data points in the matrix. For smaller 2D arrays, the minimum value of $bricks$ allowed by Felix is 2, i.e. the smallest Felix .mat file takes up 32768 bytes. One can easily determine the size (in bytes) of the .mat file from the equation

$$filesize = bricks \times 4096 \times 4$$

where there are 4K real points in a brick and 4 bytes per point.

Vectors - Following the scalar paramters, the header contains a series of “vector” parameters. These parameters are always clustered in groups of nd where nd is the number of dimensions in the matrix. For example, the first vector parameter flags the data is real or complex for each dimension. For a 2-dimensional real matrix there will be two successive 1’s stored and For a 3-dimensional real array there will be 3 successive 1’s stored. Obviously, where the storage of each vector parameter occurs in the header depends on how many matrix dimensions exist. The following table describes the vector parameters.

Table 4: Felix .mat File Header Vector Parameters

Point	Description of Vector Parameters	Values
20	Data Type for Dimension 1	1=Real, ?=Complex
21	Data Type for Dimension 2	1=Real, ?=Complex
. .	. .	. .
20+nd-1	Data Type for Dimension nd	1=Real, ?=Complex
20+nd	Number of Points in Dimension 1	
20+nd+1	Number of Points in Dimension 2	
. .	. .	. .
20+2*nd-1	Number of Points in Dimension nd	
20+2*nd	Number of Blocks in Dimension 1	1
20+2*nd+1	Number of Blocks in Dimension 2	
20+3*nd	Number of Blocks in Dimension 1	1
20+3*nd+1	Number of Blocks in Dimension 2	
20+4*nd	Blocks Size of Dimension 1 Data	1
20+4*nd+1	Blocks Size of Dimension 2 Data	

Below is a brief table of what Felix stores for its vector parameters relative to the matrix generated from the Felix bld command.

Table 5: Felix Matrices *versus* Felix Header Scalars

Felix bld Command	Vector 0	Vector 1 Points	Vector 2 Bricks	Vector 3 Brick Index	Vector 4 Blocksize	Vector 5 Block Index
bld x 2 512 512 0	1, 1	512, 512	8, 8	1, 8	64, 64	1, 64
bld x 2 512 512 1	1, 1	512, 512	8, 16	1, 8	64, 32	1, 64
bld x 2 256 512 0	1, 1	256, 512	4, 8	1, 4	64, 64	1, 64
bld x 2 512 256 0	1, 1	512, 256	8, 4	1, 8	64, 64	1, 64
bld x 2 256 512 1	1, 1	256, 512	8, 8	1, 8	32, 64	1, 32
bld x 2 512 256 1	1, 1	512, 256	8, 8	1, 8	64, 32	1, 64
bld x 2 32 1024 0	1, 1	32, 1024	2, 4	1, 2	16, 256	1, 16
bld x 2 1024 32 0	1, 1	1024, 32	4, 2	1, 4	256, 16	1, 126
bld x 2 32 1024 1	1, 1	32, 1024	4, 4	1, 4	8, 256	1, 8
bld x 2 1024 32 1	1, 1	1024, 32	4, 4	1, 4	256, 8	1, 126
bld x 3 32 32 8 0	1, 1, 1	32, 32, 8	2, 2, 1	1, 2, 4	16, 16, 16	1, 16, 256
bld x 3 32 8 32 0	1, 1, 1	32, 8, 32	2, 1, 2	1, 2, 2	16, 16, 16	1, 16, 256
bld x 3 8 32 32 1	1, 1, 1	8, 32, 32	1, 2, 2	1, 1, 2	8, 16, 16	1, 8, 128

Other Parameters - Following the vector parameters, the header contains various other parameters which track filenames, etc. The following table describes the other parameters and the last parameter in the header.

Table 6: Felix .mat File Other Parameters

Point	Description	Values
	Other	
101	Total Number of Bricks in Data (Matches Par. 2)	Includes 1 for Header
111	Number of Characters in .mat File Filename	1 <= nch <= ?
112	First Character in Filename	ASCII character
113	Second Character in Filename	ASCII character

Table 6: Felix .mat File Other Parameters

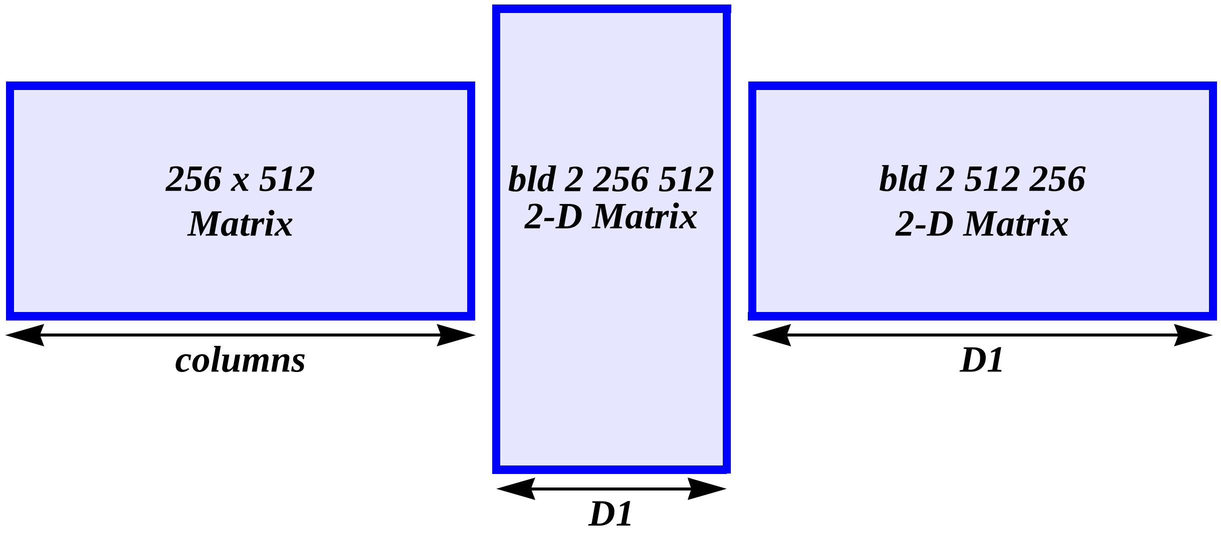
Point	Description	Values
. .	. .	. .
111+nch	Last Character in Filename	ASCII character
220	First Character of 1st Dimension Reference Text	Default = ‘D’
221	2nd Character of 1st Dimension Reference Text	Default = ‘1’
222	First Character of 2nd Dimension Reference Text	Default = ‘D’
223	2nd Character of 3rd Dimension Reference Text	Default = ‘2’
. .	. .	. .
220+nd-1	First Character of Last Dimension Reference Text	Default = ‘D’
220+nd	2nd Character of Last Dimension Reference Text	Default = nd
Last Point		
4095	Status Flag	0 = Bad, 1=Good

5.6.5 Felix ".mat" Data Structure

The matrix data points follow immediately after the Felix .mat header. These points are not stored in the typical matrix row - column fashion one is accustomed to. Rather, Felix uses an internal sub-block storage scheme which can make both matrix column and row access relatively quick[1]. We will begin this discussion talking about the more familar 2-dimensional arrays since even with these conceptually easier structures it is difficult to see what Felix is doing.

The first thing to note is that Felix does not associate its dimensions with rows or columns. This is immediately evident to anyone who has plotted a non-square array with the program. Usually, an mxn matrix is thought to contain m columns and n rows - and when sketched out on paper it appears just that way. Not so for Felix arrays! Felix plots dimension 1 horizontally and dimension 2 vertically - the exact opposite of common matrix nomenclature. This can be seen in the following diagram.

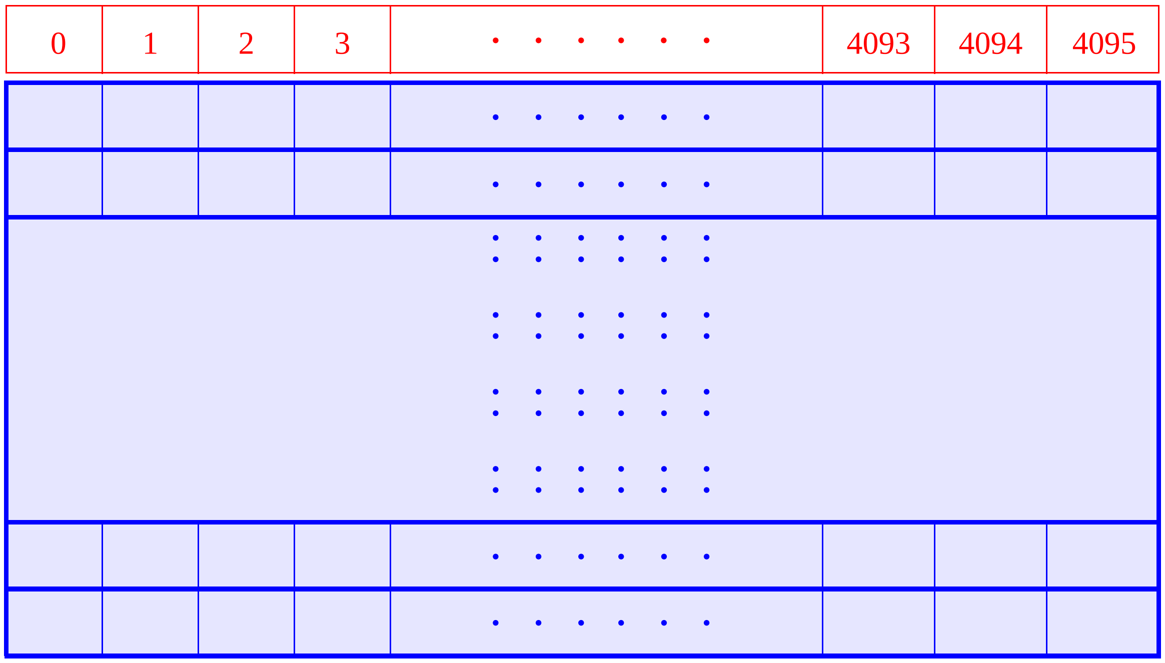
Typical Matrices versus Felix .mat 2D Matrix



Also unlike the Felix .dat file, matrix files have a **block** unit which is set to be **of length 4096** for all .mat files. Thus, the first block is the parameter header.

1. A data matrix is commonly (for example in FORTRAN) stored column-wise: <1|1>, <2|1>, <3|1>, ..., <n|1>, <2|1>, <2|2>, ... <n|n>. Accessing a column with this storage scheme needs one disk seek followed by successive elements being rapidly read. Accessing a row then requires a disk seek for each element and is thus much slower. (For a matrix stored row-wise the opposite logic holds.) By using a sub-matrix storage scheme, both row and column access will be faster that the row read of the typically stored matrix, the tradeoff being both are slower that row read of common storage method. The bottom line is that if you assume you will be processing both rows and columns of the matrix a lot the latter storage will always seem reasonably fast whereas the simpler storage will probably seem unbearably slow whenever the less favorable access is needed..

General Felix .mat File Structure



There is also a larger structure in the matrix files, called a **brick**, which clusters together several blocks. A brick is used to easily jump from one matrix point to the next in any of the matrix dimensions. We will use two examples to illustrate the brick/block matrix structures. The following figure outlines the storage of a matrix constructed by the Felix command *bld x 2 512 512 0*. Felix stores these points in 64 point clumps, the first clump belonging to elements which would be read by the Felix command *loa 0 1* (a row in standard matrix nomenclature). The the next clump contains the first 64 elements which would be read by *loa 0 2*, and so on until the entire 4K block is filled up. It is the second block which contains the second set of 64 point clumps for all of these (rows) and since dimension 1 spans 512 points it takes 8 complete blocks to span the vectors obtained by *loa 0 1* through *loa 0 64*. This is a brick. The data obtained from *loa 0 65* begins at the start of the second brick, at the 8th block (0-7 allotted to brick 0).

Felix .mat File Structure for 512x512 Real Matrix

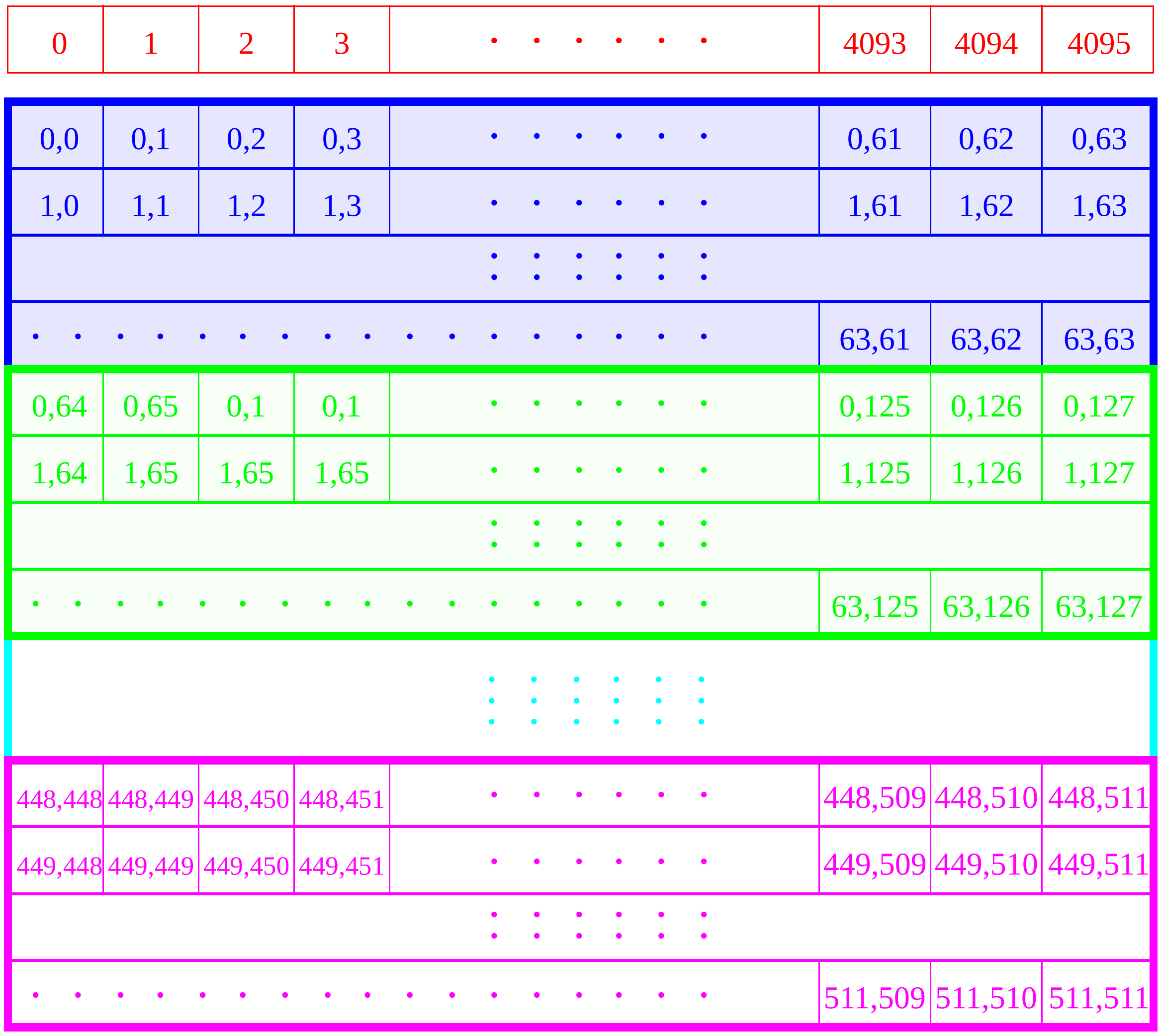


Figure 4-11 - Header Structure of an Felix .mat file. Note that the index in FORTRAN (the language in which Felix is written) is shifted by +1 realative to the standard C indexing used in GAMMA, that is vectors start at 21 and end at 100, etc.

Below is a brief table of the first for scalar parameters found versus the matrix generated from the Felix bld command.

Table 7: Felix Matrices *versus* Felix Header Scalars

Felix bld Command	Scalar 0 Dimensions	Scalar 1 Type	Scalar 2 Bricks	Scalar 3 Blocks	Matrix Filesize	Matrix Points
bld test 2 512 512 0	2	1	65	8	1064960	262144
bld test 2 512 512 1	2	2	129	16	2113536	524288

Table 7: Felix Matrices *versus* Felix Header Scalars

Felix bld Command	Scalar 0 Dimensions	Scalar 1 Type	Scalar 2 Bricks	Scalar 3 Blocks	Matrix Filesize	Matrix Points
bld test 2 256 512 0	2	1	33	8	540672	131072
bld test 2 512 256 0	2	1	33	8	540672	131072
bld test 2 256 512 1	2	2	65	8	1064960	524288
bld test 2 512 256 1	2	2	65	8	1064960	524288
bld test 2 32 1024 0	2	1	9	4	147456	32768
bld test 2 1024 32 0	2	1	9	4	147456	32768
bld test 2 32 1024 1	2	2	17	4	278528	65536
bld test 2 1024 32 1	2	2	17	4	278528	65536
bld test 3 32 32 8 0	3	1	5	2	81920	8192
bld test 3 32 8 32 0	3	1	5	2	81920	8192
bld test 3 8 32 32 1	3	2	5	2	81920	16384

As seen from the above table, the number of stored dimensions and the matrix data type is straightforward. The number of bricks which felix uses can be determined by the formula

$$bricks = [(rpts/4096) + 1]$$

where $rpts$ is the total number of real points in the matrix. The minimum value of $bricks$ allowed by felix is 5, i.e. the smallest Felix .mat file takes up 81920 bytes. One can easily determine the size of the .mat file from the following equation,

$$filesize = bricks \times 4096 \times 4$$

where there are 4K real points in a brick and 4 bytes per point.

Below is a brief table of what Felix stores for its vector parameters relative to the matrix generated from the Felix bld command.

Table 8: Felix Matrices *versus* Felix Header Scalars

Felix bld Command	Vector 0	Vector 1 Points	Vector 2 Bricks	Vector 3 Brick Index	Vector 4 Blocksize	Vector 5 Block Index
bld x 2 512 512 0	1, 1	512, 512	8, 8	1, 8	64, 64	1, 64
bld x 2 512 512 1	1, 1	512, 512	8, 16	1, 8	64, 32	1, 64
bld x 2 256 512 0	1, 1	256, 512	4, 8	1, 4	64, 64	1, 64

Table 8: Felix Matrices *versus* Felix Header Scalars

Felix bld Command	Vector 0	Vector 1 Points	Vector 2 Bricks	Vector 3 Brick Index	Vector 4 Blocksize	Vector 5 Block Index
bld x 2 512 256 0	1, 1	512, 256	8, 4	1, 8	64, 64	1, 64
bld x 2 256 512 1	1, 1	256, 512	8, 8	1, 8	32, 64	1, 32
bld x 2 512 256 1	1, 1	512, 256	8, 8	1, 8	64, 32	1, 64
bld x 2 32 1024 0	1, 1	32, 1024	2, 4	1, 2	16, 256	1, 16
bld x 2 1024 32 0	1, 1	1024, 32	4, 2	1, 4	256, 16	1, 126
bld x 2 32 1024 1	1, 1	32, 1024	4, 4	1, 4	8, 256	1, 8
bld x 2 1024 32 1	1, 1	1024, 32	4, 4	1, 4	256, 8	1, 126
bld x 3 32 32 8 0	1, 1, 1	32, 32, 8	2, 2, 1	1, 2, 4	16, 16, 16	1, 16, 256
bld x 3 32 8 32 0	1, 1, 1	32, 8, 32	2, 1, 2	1, 2, 2	16, 16, 16	1, 16, 256
bld x 3 8 32 32 1	1, 1, 1	8, 32, 32	1, 2, 2	1, 1, 2	8, 16, 16	1, 8, 128

6 NMRi I/O

6.1 Overview

The NMRi I/O routines are provided to allow the transfer of data between GAMMA and the programs NMR1 and NMR2[1].

6.2 Available NMRi Functions

6.3 Routines

6.3.1 NMRi

Usage:

```
#include <NMRi.h>
void NMRi (const char* filename, block_1D &BLK, int rc=1);
void NMRi (const char* filename, block_2D &BLK, int rc=1);
void NMRi (File &file, block_1D &BLK, int rc=1, int zero=0);
```

Description:

The function NMRi is used to write files in the standard NMRi format. The data is contained in the data block "BLK". The file is specified by either the name "filename" or by the file pointer "file". The parameter "rc" indicates whether to write real or complex(default) data. If rc is 0, only the real data will be output. If rc is negative, only the imaginary data is written (as reals), and if rc>0 the complex data is written.

1. NMRi (const char* filename, block_1D &BLK, int rc=1) - When NMRi is invoked with this argument list it writes the data contained in the 1-dimensional data block "BLK" to a newly constructed file "filename" in the NMRi format. If rc is 1 (default) the data is written as complex numbers. If rc is set to zero, only the real data of the block is output. Any parameters in BLK compatible with the NMRi parameters will be automatically transferred into the NMRi file. The file is closed upon the function return. The func-

1. NMR1 and NMR2 are a products of New Methods Research, Inc., 7 East Genesee Street, Syracuse, NY, 13210. Phone: (315) 424-0329, FAX: (315) 424-0356.GAMMA was tested on Sun systems running the Sunviews operating system. NMR1 release 3.8 and NMR2 release 3.5 were the manuals referred to during the programming.

tion will overwrite any file “filename” previously in existence. No other NMRi file should be open during the calling of this function.

2. NMRi (const char* filename, block_2D &BLK, int rc=1) - This function is similar to the use above (with 1D data blocks) but writes the data contained in the 2-dimensional data block “BLK”. This is done row-wise, i.e. first row 1 of BLK is written followed by row 2 and so on until the end of the data in BLK.
3. NMRi (File &file, block_1D &BLK, int rc=1) - When NMRi is invoked with this argument list it writes the data contained in the 1-dimensional data block “BLK” in the NMRi format to wherever the file pointer “file” is at. The file where “file” is pointing is assumed to be open (opened explicitly sometime prior to the function call) and will remain open with the file pointer advanced to the file end at the function return. The file should be closed externally as well. The NMRi parameter block is updated with each function call. An optional parameter in this function is “zero” which, if non-zero, will set the count of 1D spectra present in the NMRi file to zero. This is done automatically in most instances but should be used if multiple NMRi files are to be produced in a single program run it is necessary to re-zero the count when writing the first spectrum of all NMRi files.

Note that NMRi can be called with a matrix instead of a block_2D or a row_vector rather than a block_1D. In these instances the parameter sets are not fully written into the NMRi file.

Return Value:

Nothing when producing a NMRi file.

Example:

```
#include <gamma.hc>
main ()
{
 block_1D BLK1(128);                    // Define a 1D-data block
BLK1 = Gaussian(128, 64, 42.46);        // Set 1D-block to Gaussian
NMRi(“NMR1D.tst”, BLK1);                // Output 1D BLK to NMRi file
block_2D BLK2(128,128);                 // Define a 2D-data block
for(int i=0; i<128; i++)                // Fill 2D block with 2D-Gaussian
  for(int j=0; j<128; j++)
    BLK2(i,j) = BLK1(i)*BLK1(j);
NMRi(“NMR2D.tst”, BLK2);                // Output 2D BLK to NMRi file
File fp;                                // Specify a file pointer
fp.open(“NMRND.tst”,io_writeonly
                            ,a_create); // Open file NMRND.tst
block_1D BLKA(128), BLKB(128);          // Define two more 1D-data blocks
BLKA = sinc(128, 64, 12);               // Set block to sinc function
BLKB = 127-i * BLK1;
NMRi(fp, BLKB, 0, 1);                   // Last 1 needed as previous NMRi files used
for(i=1; i<128; i++)                    // Output 128 1D blocks to NMRi file
  {                                     // only the reals are output here
  BLKB = i*BLKA + (127-i)*BLK1;
  NMRi(fp, BLKB, 0);
  }
fp.close();                              // Close file NMRND.tst
}
```

The last NMRi file produced, NMRND.tst, was made by first opening a file, successively writing 1D spectra to it, then closing the file. Since this program accessed NMRi files previously (during the creation of NMR1D.tst and NMR2D.tst) the first spectrum was independently written outside the loop with the zero flag set when calling NMRi. This sets the internal counter to zero, something unnecessary had NMRi files not been previously created in the program.

6.3.2 NMRi_1D

Usage:

```
#include <NMRi.h>
block_1D NMRi_1D (const char* filename, int spectrum=1);
```

Description:

The function NMRi_1D is used to read a 1D spectrum from an NMRi file, that is, a file in the standard NMRi format. The NMRi file name is “filename”. Returned is an 1D-data block containing the parameters in the NMRi file along with the spectrum chosen with “spectrum”. The default spectrum will be the initial one.

Return Value:

A one dimensional data block.

Example:

6.3.3 NMRi_2D

Usage:

```
#include <NMRi.h>
block_2D NMRi_2D (const char* filename);
```

Description:

The function NMRi_2D is used to read a 2D spectrum from an NMRi file, that is, a file in the standard NMRi format. The NMRi file name is “filename”. Returned is an 2D-data block containing the parameters in the NMRi file along with the entire 2D spectrum.

Return Value:

A two dimensional data block.

Example:

6.3.4 NMRi_header

Usage:

```
#include <NMRi.h>
ostream& NMRi_header (const char* filename, int verbose=0);
```

Description:

The function NMRi_header is used to quickly read the header information contained in an NMRi file. The NMRi file name is “filename”. The header contains 512 pieces of information, only some of which is particularly useful outside of the NMRi programs themselves. The integer verbose specifies how much of this information should be returned. The default value of 0 returns the minimal amount of information, the amount increases as verbose increases up to 10. The header is returned in an output stream.

Return Value:

None, the function sends information to standard output

Example:

```
#include <gamma.h>

main ()
{
String filename;                        // Declare a string
cout << “Which Levy File ?”;            // Ask for filename
cin >> filename;                        // Input filename
int verbose;                            // Declear an integer
cout << “\nHow verbose ?”;              // Ask for verbose level
cin >> verbose;                         // Input verbose level
cout << “\n\n”;                         // Output line feed (so screen is nice)
NMRi_header(filename, verbose);         // Output the header info in filename
}
```

In this example, the user is queried for the file and the amount of information should be returned. The default value of 0 returns the minimal amount of information, the amount increases as verbose increases up to 10. The header information is returned to the standard output stream.

6.4 Description

NMRi File Structure - NMRi files begin with a header which contains 512 parameters describing the spectral data. A 1D-spectrum of length "SIZE" is written immediately after the header, all real values followed by all imaginary values. If the data is not complex, the imaginary values are absent from the file. A two (or multi-) dimensional spectrum is successive 1D-spectra sharing the same header information, as depicted in the figure below.

NMRi File Structure

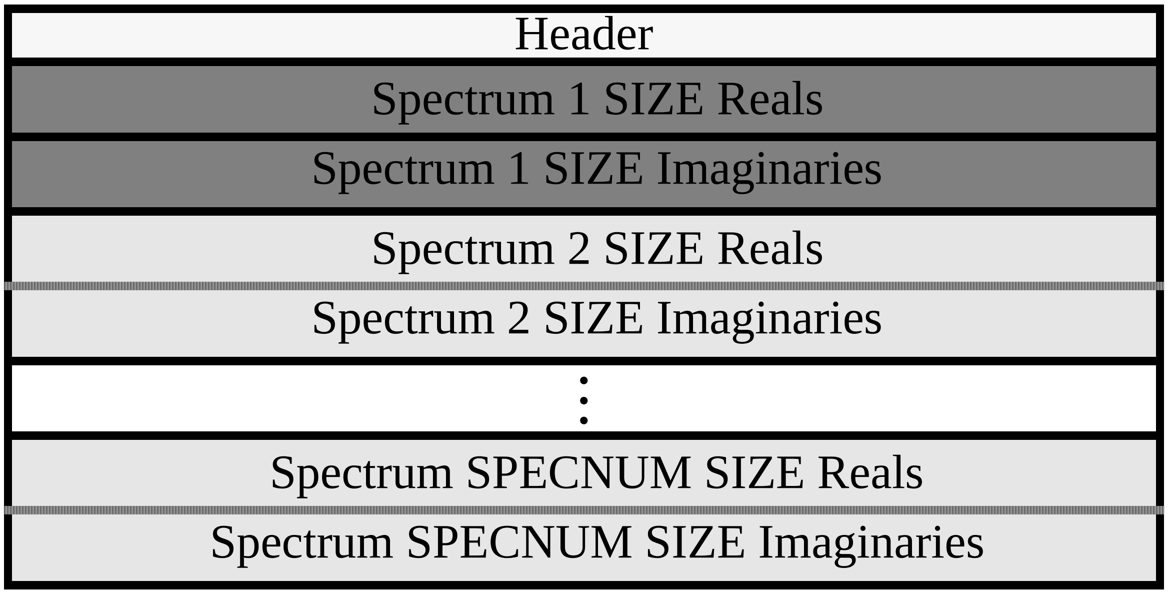

Header
Spectrum 1 SIZE Reals
Spectrum 1 SIZE Imaginaries
Spectrum 2 SIZE Reals
Spectrum 2 SIZE Imaginaries
Spectrum SPECNUM SIZE Reals
Spectrum SPECNUM SIZE Imaginaries

Figure 25-1 - Overall file structure of a NMRi file containing SPECNUM 1D complex spectra each of length SIZE.

This file structure is described in the NMRi manual *LAB ONE NMR2*, USER MANUAL, Release 3.5 on page 29.

NMRi Header Structure - A full listing of the parameters contained in the header is given in the NMRi manual *LAB ONE NMR1*, USER MANUAL, Release 3.8 on page 1-37. Of the 512 parameters it contains, few are useful outside of the NMRi programs. Those absolutely required are given in the NMR2 manual (cited previously) on page 28 and listed here.

• 100	- First dimension size. This is SIZE in Figure 25-1
• 101	- First dimension spectral width.
• 107	- Data type: 0.0=quadrature, 1.0=singulature, 2.0=singulature sorted.
• 220	- Second dimension size. This is SPECNUM in Figure 25-1
• 230	- Second dimension spectral width.

For consistency with the program description found in the supplied manuals, the file structure will be briefly discussed in terms of blocks, each block being of length 64[1]. Thus the header takes up 4 blocks.

NMRi Header Structure

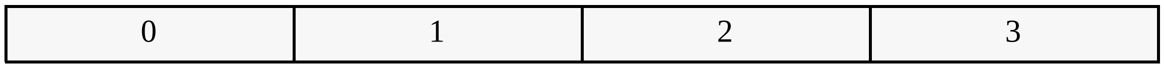


Figure 25-2 - Header Structure of a NMRi file. The header is conceptually divided into 4 blocks, each containing 64 parameters.

NMRi Data Structure - The actual data starts immediately after the header. In a file containing multiple spectra (i.e. a 1D spectrum) each spectrum must be of the same size and this size must be a power of 2 (64, 128, 256, ...). If the any spectrum does not meet this latter requirement it will be padded with zeros until the size is a power of 2. Furthermore, they must all be real or all be complex.

NMRi Data Structure

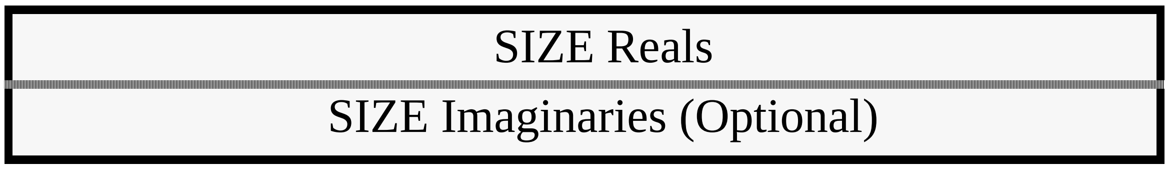


Figure 25-3 - Structure of NMRi 1D-spectrum.

Again, for consistency with the program description found in the supplied manuals, the file structure will be discussed in terms of blocks of length 64[2]. The data begins at block number 4, and the length of each 1D-spectrum will be

$$LENGTH = (SIZE)/64$$

for a complex data set where LENGTH is given in blocks. For a real data set, this number will be halved.

GAMMA - When creating NMRi files, GAMMA will initially write an empty header (512) prior to any spectral data. After each 1D-spectrum is written, the header will be updated to reflect how many lines of 1D data are present. That would be the variable SPECNUM shown in Figure 25-1.

1. The block length of 64 is intrinsic to the file structure as utilized in the FORTRAN code for file I/O supplied with the NMRi programs.GAMMA uses C++ code to perform I/O withe NMRi making this conceptual division nearly unnecessary.
2. See the previous footnote. This information is only useful in clarification of the manual description.

7 NMRiFile

7.1 Overview

The class NMRiFile provides I/O functions to read and write files in NMRi Format. This class is constructed in analogy to the standard C++ class File for handling files on disk. As such, each NMRiFile accesses a disk file, either for reading or writing. Provisions are made for transferring the data in an NMRiFile into a matrix or from a matrix into an NMRiFile.

7.2 Available NMRiFile Functions

7.3 NMRiFile Figures and Tables

7.4 Routines

7.4.1 NMRiFile

Usage:

```
#include <NMRiFile.h>
void NMRi (const char* filename, io_mode m=io_readwrite, access_mode a=a_use);
```

Description:

The function ***NMRiFile*** is used to either create a new NMRi compatible file or to open an existing file which is in the standard NMRi format. The first argument, ***filename***, is the NMRi file name to be accessed. The second argument, ***io_mode*** is exactly analogous to the valid arguments used to open a file. The possible input values are: io_readonly - the file will be opened without write access, io_writeonly - the file will be open for writing only, io_readwrite - the file will be opened for both reading and writing (default). The last argument, ***access_mode***, is also analogous to access modes for files. The possible input values are: a_createonly - create the file, fail if file exists; a_create - create the file, recreate if file exists; a_useonly - open an existing file, fail if it does not exist; a_use - open an existing file, create if it does not exist. The default values of the latter two are usually correct but the NMRi file must then have both read and write privileges set for the individual attempting to access it.

Return Value:

Nothing when producing a NMRi file.

Example:

```
#include <NMRiFile.h>
main ()
 {
 NMRiFile file1("newfile.dat");          // Create a new NMRiFile file1, external name newfile.dat
 NMRiFile file2("oldfile.dat");          // Open an old NMRiFile file2, external name oldfile.dat
 }
```

7.4.2 close

Usage:

```
#include <NMRiFile.h>
void NMRi (const char* filename, io_mode m=io_readwrite, access_mode a=a_use);
```

Description:

The function NMRiFile is used to either create a new NMRi compatible file or to open an existing file which is in the standard NMRi format. The data is contained in the data block "BLK". The file is specified by either the name "filename" or by the file pointer "file". The parameter "rc" indicates whether to write real or complex(default) data. If rc is 0, only the real data will be output. If rc is negative, only the imaginary data is written (as reals), and if rc>0 the complex data is written.

Return Value:

Nothing when producing a NMRi file.

Example:

```
#include <gamma.hc>
main ()
{
 block_1D BLK1(128);                   // Define a 1D-data block
BLK1 = Gaussian(128, 64, 42.46);       // Set 1D-block to Gaussian
  NMRi(fp, BLKB, 0);
  }
fp.close();                            // Close file NMRND.tst
}
```

The last NMRi file produced, NMRND.tst, was made by first opening a file, successively writing 1D spectra to it, then closing the file. Since this program accessed NMRi files previously (during the creation of NMR1D.tst and NMR2D.tst) the first spectrum was independently written outside the loop with the zero flag set when calling NMRi. This sets the internal counter to zero, something unnecessary had NMRi files not been previously created in the program.

7.4.3 write

Usage:

```
#include <NMRiFile.h>
void write (const matrix& mx);
void write (const block_1D& BLK);
void write (const block_2D& BLK);
```

Description:

The function ***write*** is used to write data from a GAMMA matrix (or block) into an NMRi compatible file. There is only one argument and it can be either a matrix, 1-dimensional data block, or 2-dimensional data block.

Return Value:

Nothing the function is void. The NMRi file will be modified.

Example:

```
main ()
  {
  NMRiFile file1(“oldfile.dat”);       // Open an old NMRiFile file1, external name oldfile.dat
  mstrix mx;                           // Declare a general matrix
  block_1D BLK1;                       // Declare a 1D data block
  block_2D BLK2;                       // Declare a 2D data block
```

```
 file1.read(mx);                // Read all the data points in oldfile.dat into matrix mx
 file1.read(BLK2);              // Read all data points in oldfile.dat into 2D block BLK2
 }
```

7.4.4 read

Usage:

```
#include <NMRiFile.h>
void read (matrix& mx);
void read (block_1D& BLK);
void read (block_2D& BLK);
void read (matrix& mx, int rows);
void read (block_1D& BLK, int rows);
void read (block_2D& BLK, int rows);
```

Description:

The function ***read*** is used to read data from an NMRi compatible file into a GAMMA matrix (or data block). Only one argument in utilized in the first three funciton forms, either a matrix, 1-dimensional data block, or 2-dimensional data block. With this usage, the

Return Value:

Nothing the function is void. The NMRi file will not be modified.

Example:

```
#include <NMRiFile.h>
main ()
 {
 NMRiFile file1("oldfile.dat");   // Open an old NMRiFile file1, external name oldfile.dat
 mstrix mx;                       // Declare a general matrix
 block_1D BLK1;                   // Declare a 1D data block
 block_2D BLK2;                   // Declare a 2D data block
 file1.read(mx);                  // Read all the data points in oldfile.dat into matrix mx
 file1.read(BLK2);                // Read all data points in oldfile.dat into 2D block BLK2
 }
```

7.4.5 writeParameter

Usage:

```
#include <NMRiFile.h>
void NMRiFile::writeParameter (int pos, mx, float par);
void NMRiFile::writeParameter (int pos, int par);
```

Description:

The function ***writeParameter*** is used to write parameters into an NMRiFile. For this function the value of the argument ***pos*** indicates which parameter, relative to the beginning of the file, is to be written. The value of the parameter itself, ***par***, can be input as either a floating point number or an integer.

Return Value:

Nothing the function is void. The NMRi file will be modified by having the parameter specified altered.

Example:

```
#include <NMRiFile.h>
main ()
{
                              ,a_create);   // Open file NMRND.tst
}
```

7.4.6 readParameter

Usage:

```
#include <NMRiFile.h>
void NMRiFile::readParameter (int pos, mx, float& par);
void NMRiFile::readParameter (int pos, int& par);
```

Description:

The function ***readParameter*** is used to read parameters from an NMRiFile. For this function the value of the argument ***pos*** indicates which parameter, relative to the beginning of the file, is to be written. The value of the parameter, ***par***, will be set and output as either a floating point number or an integer type depending on the argument given.

Return Value:

Nothing the function is void. The value of input parameter will be set the NMRi parameter.

Example:

```
#include <NMRiFile.h>
main ()
 {
 NMRiFile file1("oldfile.dat");          // Open an old NMRiFile file1, external name oldfile.dat
 cout << “No. of rows = file1.rows();     // Output the number of rows contained in the file
 }
```

7.4.7 write_header

Usage:

```
#include <NMRiFile.h>
void NMRiFile::write_header();
```

Description:

The function ***write_header*** is used to write all 512 parameters into an NMRi file into a floating point array. The NMRi file will be accessed directly regardless of where the file pointer is. The file pointer will be immediately after the header, at the start of the data.

Return Value:

This function returns a pointer to a floating point array.

Example:

```
#include <NMRiFile.h>
main ()
 {
 NMRiFile file1(“newfile.dat”);          // Open an new NMRiFile file1, external name newfile.dat
 float fdata[512]                        // Declare a float array of 512 points
 file1.write_header(fdata);              // Write all 512 parameters in fdata to file1’s header
 }
```

7.4.8 read_header

Usage:

```
#include <NMRiFile.h>
float* NMRiFile::read_header();
```

Description:

The function ***read_header*** is used to read all 512 parameters contained in an NMRi file into a floating point array. The NMRi file will be accessed directly regardless of where the file pointer is. The file pointer will be immediately after the header, at the start of the data.

Return Value:

This function returns a pointer to a floating point array.

Example:

```
#include <NMRiFile.h>
main ()
 {
```

```
 NMRiFile file1(“oldfile.dat”);          // Open an old NMRiFile file1, external name oldfile.dat
 float* fdata                            // Declare a pointer to a float
 fdata = oldfile.read_header();          // Now fdata is an array filled with  all header parameters
 }
```

7.4.9 print_header

Usage:

```
#include <NMRiFile.h>
ostream& NMRiFile::print_header(ostream& ostr, int level=1);
```

Description:

The function ***print_header*** is used to send the parameter information contained in an NMRi file header into an output stream. The returned output stream is the stream given in the first argument, ostr, with the header parameters added. The second argument, level, set the amount of parameters to include in the output. The range of level = [1, 5] where 1 outputs only the essential parameters of the possible 512 values.

Return Value:

This function returns an output stream.

Example:

```
#include <NMRiFile.h>
main ()
 {
 NMRiFile file1(“oldfile.dat”);          // Open an old NMRiFile file1, external name oldfile.dat
 cout << file1.print_header(cout);       // Output the basic header parameters
 }
```

7.4.10 rows

Usage:

```
#include <NMRiFile.h>
int NMRiFile::rows ( );
```

Description:

The function ***rows*** is used to obtain the number of rows (or data blocks) the NMRi file contains.

Return Value:

An integer is returned.

Example:

```
#include <NMRiFile.h>
main ()
 {
```

```
 NMRiFile file1("oldfile.dat");            // Open an old NMRiFile file1, external name oldfile.dat
 cout << "No. of rows = file1.rows();      // Output the number of rows contained in the file
 }
```

7.4.11 cols

Usage:

```
#include <NMRiFile.h>
int NMRiFile::cols ( );
```

Description:

The function ***cols*** is used to obtain the number of points that each row (or data blocks) of the NMRi file contains.

Return Value:

An integer is returned.

Example:

```
#include <NMRiFile.h>
main ()
 {
 NMRiFile file1("oldfile.dat");            // Open an old NMRiFile file1, external name oldfile.dat
 cout << "No. of columns = file1.cols(); // Output the number of columns contained in the file
 }
```

7.4.12 seek

Usage:

```
#include <NMRiFile.h>
void NMRiFile::seek (int pos, int seek_mode=0);
```

Description:

The function ***seek*** is used to set the internal positioning in the NMRi file. The argument ***pos*** is a value for the position in rows (or data blocks). The second argument ***seek_mode*** indicates how ***pos*** is implemented. The default value, ***seek_mode*** = 0, the file position is set at ***pos*** rows from the file start. For the value ***seek_mode*** =1 the file position is set +***pos*** rows from the current position. For the value ***seek_mode*** =2 the file position is set ***pos*** rows back from the end of the file.

Return Value:

None, the function is void.

Example:

```
#include <NMRiFile.h>
main ()
```

```
 {
 NMRiFile file1("oldfile.dat");        // Open an old NMRiFile file1, external name oldfile.dat
 file1.seek(5);                        // Skip to row 5 of the data in file1
 file1.seek(2, 2);                     // Skip to the second row 5 from the end of the data in file1
 file1.seek(1);                        // Skip one row (now to last one)
 }
```

7.4.13 tell

Usage:

```
#include <NMRiFile.h>
int NMRiFile::tell ( );
```

Description:

The function ***tell*** is used to obtain the current file position, in terms of rows (or blocks) of an NMRi file.

Return Value:

An integer is returned.

Example:

```
#include <NMRiFile.h>
main ()
 {
 NMRiFile file1("oldfile.dat");        // Open an old NMRiFile file1, external name oldfile.dat
 file1.seek(5);                        // Skip to row 5 of the data in file1
 file1.seek(2, 2);                     // Skip to the second row 5 from the end of the data in file1
 file1.seek(1);                        // Skip one row (now to last one)
 }
```

7.4.14 =

Usage:

```
#include <NMRiFile.h>
int NMRiFile::tell ( );
```

Description:

The function = is used to place all parameters contained in the NMRi file header into a parameter set (***class p_set***).

Return Value:

Void.

Example:

```
#include <NMRiFile.h>
```

```
main ()
 {
 NMRiFile file1("oldfile.dat");          // Open an old NMRiFile file1, external name oldfile.dat
 file1.seek(5);                          // Skip to row 5 of the data in file1
 file1.seek(2, 2);                       // Skip to the second row 5 from the end of the data in file1
 file1.seek(1);                          // Skip one row (now to last one)
 }
```

7.5 Class NMRiFile Description

7.5.1 Introduction

Every data file suitable for use in the NMR data processing packages from New Methods Research, Inc.[1] (e.g. NMR1 and NMR2) has a standard internal format. ***Class NMRiFile*** was constructed in order that users of GAMMA are able to efficiently manipulate such files.

7.5.2 NMRiFile Structure

The internal design of ***Class NMRiFile*** is quite simple. It contains the quantities defined in the following table.

Table 9: NMRiFile Internal Structure

Variable	Type	Units	Description	Comments
fp	File		The NMRi file on disk	Set in constructor
fsize	int	bytes	Size of NMRi file in bytes	
cols_	int	points	Number of columns in the file	
row_	int	points	Number of rows in the file	
pos_	int	bytes	Current position in file	
fname	String		External NMRi file name	Set in constructor
headersize	int	parame-ters	Size of NMRi file header	Set Constant: 512
par_SIZE	int	parame-ters	File position of parameter SIZE	Set Constant: 99
par_SPEC S	int	parame-ters	File position of parameter SPECS	Set Constant: 219

Most manipulations within ***NMRiFile*** are performed with the C++ class ***File***. The other quantities are defined mostly for convenience and/or because they are constants for all NMRi files.

1. NMR1 and NMR2 are a products of New Methods Research, Inc., 7 East Genesee Street, Syracuse, NY, 13210. Phone: (315) 424-0329, FAX: (315) 424-0356.GAMMA was tested on Sun systems running the Sunviews operating system. NMR1 release 3.8 and NMR2 release 3.5 were the manuals referred to during the programming.

7.5.3 NMRi File Structure

NMRi files begin with a header which contains 512 parameters (headersize) describing the spectral data. A 1D-spectrum of length “SIZE” is written immediately after the header, all real values followed by all imaginary values. If the data is not complex, the imaginary values are absent from the file. A two (or multi-) dimensional spectrum is successive 1D-spectra sharing the same header information, as depicted in the figure below.

NMRi File Structure

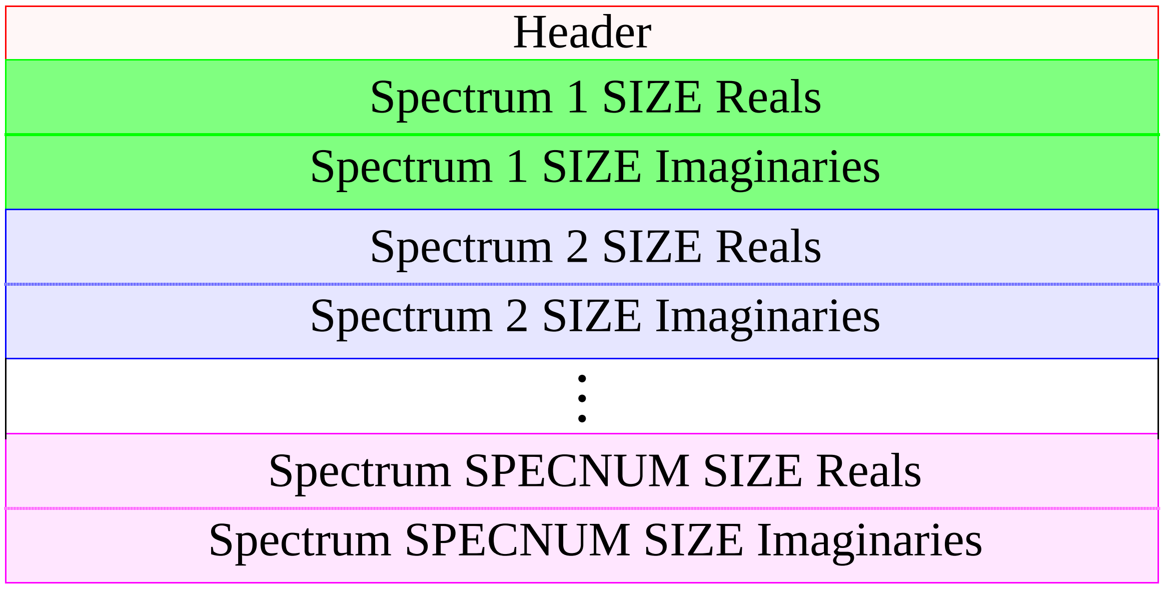

Header
Spectrum 1 SIZE Reals
Spectrum 1 SIZE Imaginaries
Spectrum 2 SIZE Reals
Spectrum 2 SIZE Imaginaries
Spectrum SPECNUM SIZE Reals
Spectrum SPECNUM SIZE Imaginaries

Figure 29-1 - Overall file structure of a NMRi file containing SPECNUM 1D complex spectra each of length SIZE.

This file structure is described in the NMRi manual *LAB ONE NMR2*, USER MANUAL, Release 3.5 on page 29.

7.5.4 NMRi Header Structure

A listing of the parameters contained in the header is given in the *NMR1* USER MANUAL, Appendix F and also in the *NMR2* USER MANUALR, Appendix A. The parameters discussed in the two sources do not coincide exactly but the descriptions are suitable for GAMMA purposes. Of the 512 parameters contained in the header, few are useful outside of the NMRi programs. Those absolutely required are given in the NMR2 manual (see the beginning section Data File Format) and listed here. Note that here numbers range from 1 to 512 (not [0,511]).

• 100	- First dimension size. This is SIZE in Figure 29-1
• 101	- First dimension spectral width.
• 107	- Data type: 0.0=quadrature, 1.0=singulature, 2.0=singulature sorted.
• 220	- Second dimension size. This is SPECNUM in Figure 29-1
• 230	- Second dimension spectral width.

Other parameters which should be included, according to the NMR2 manual, are the following.

• 120	- Spectrometer Frequency (F2 Observe Frequency).
• 153	- First Dimension Units.
• 219	- Spectrometer Frequency (F1 Observe Frequency).
• 221	- First Dimension Transform State.
• 222	- Transpose State
• 223	- Second Dimensiton Transform State.
• 235	- Second Dimension Units.

For consistency with the program description found in the supplied manuals, the file structure will be briefly discussed in terms of blocks, each block being of length 64[1]. Thus the header takes up 4 blocks.

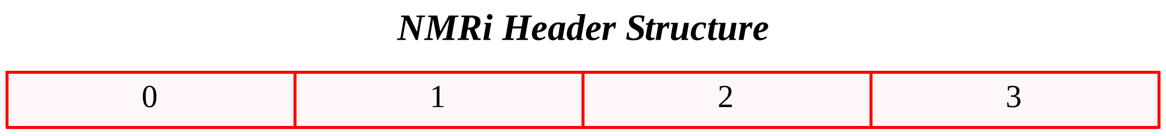


Figure 29-2 - Header Structure of a NMRi file. The header is conceptually divided into 4 blocks, each containing 64 parameters.

1. The block length of 64 is intrinsic to the file structure as utilized in the FORTRAN code for file I/O supplied with the NMRi programs. GAMMA uses C++ code to perform its I/O regarding NMRi files rendering this conceptual division unnecessary.

7.5.5 NMRi Data Structure

The actual data starts immediately after the header. In a file containing multiple spectra (i.e. a 2D spectrum) each spectrum must be of the same size and this size must be a power of 2 (64, 128, 256, ...). If the any spectrum does not meet this latter requirement it will be padded with zeros until the size is a power of 2. Furthermore, collectively the blocks must be either all real or all complex.

NMRi Data Structure

SIZE Reals
SIZE Imaginaries (Optional)

Figure 29-3 - Structure of NMRi 1D-spectrum or block.

Again, for consistency with the program description found in the supplied manuals, the file structure will be discussed in terms of blocks of length 64[1]. The data begins at block number 4, and the length of each 1D-spectrum will be

$$LENGTH = (SIZE)/64$$

for a complex data set where LENGTH is given in blocks. For a real data set, this number will be halved.

7.5.6 GAMMA Treatment of NMRi Files

When creating NMRi files, GAMMA will initially write an empty header (512) prior to any spectral data. After each 1D-spectrum is written, the header will be updated to reflect how many lines of 1D data are present. That would be the variable SPECNUM shown in Figure 29-1.

1. See the previous footnote. This information is only useful in clarification of the manual description.